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Summary

The subject of this Ph.D.-thesis is somewhere in between continuous and discrete geometry.

Chapter 2 treats the geometry of finite point sets in semi-Riemannian hyperquadrics, using a matrix whose entries are a trigonometric function of relative distances in a given point set. The distance introduced on the semi-Riemannian space forms has complex values and is an extension of the usual Riemannian distance on the simply connected space forms.

One of the most important results of the chapter is Theorem 2, that relates the determinant of the previously mentioned trigonometric matrix to the geometry of a simplex in a semi-Riemannian hyperquadric.

In chapter 3 we study which finite metric spaces that are realizable in a hyperbolic space in the limit where curvature goes to $-\infty$. We show that such spaces are the so called *leaf spaces*, the set of degree 1 vertices of weighted trees.

We also establish results on the limiting geometry of such an isometrically realized leaf space simplex in hyperbolic space, when curvature goes to $-\infty$.

Chapter 4 discusses *negative type* of metric spaces. We give a measure theoretic treatment of this concept and related invariants. The theory developed is then applied to show, that hyperbolic spaces are of strictly negative type. We also give an application to maximal distributions of subharmonic kernels.

The most important application is probably the discussion of closed geodesics and negative type. Among other things we show, that a compact Riemannian manifold of negative type and dimension at least 2 is simply connected.

Dansk resumé

Emnet for denne Ph.d.-afhandling er et sted i mellem kontinuert og diskret geometri, med skiftende fokus.

Kapitel 2 beskriver geometrien af endelige punktmængder i konstant krummede semi-Riemannske mangfoldigheder, med udgangspunkt i en matrix, hvor indgangene er en trigonometrisk funktion af indbyrdes afstande i punktmængden. Afstanden vi indfører på disse mangfoldigheder har komplekse værdier og er en generalisering af den klassiske Riemannske afstand på de enkeltsammenhængende konstant krummede rum.

Et af kapitlets vigtigste resultater er Theorem 2, der relaterer determinanten af den føromtalte trigonometriske matrix, til geometrien af et simplex i en semi-Riemannsk rumform.

I kapitel 3 undersøger vi hvilke metriske rum, der kan indlejres i et hyperbolsk rum i grænsen hvor krumning går mod $-\infty$. Det vises at sådanne metriske rum netop er de såkaldte bladrum, der består af knuder med grad 1 i et endeligt metrisk træ.

Vi etablerer også resultater omkring konvergensen af geometrien af det indlejrede rum, når krumningen går imod $-\infty$.

Kapitel 4 omhandler *negativ type* af metriske rum. Vi giver en målteoretisk diskussion af dette begreb og relaterede invarianter. Den udviklede teori anvendes til at vise, at hyperbolske rum er af streng negativ type. Desuden gives en anvendelse for subharmoniske *kerner*. Den vigtigste anvendelse er dog nok diskussionen af lukkede geodæter i kompakte mangfoldigheder af negativ type. Vi viser blandt andet, at en kompakt Riemannsk mangfoldighed af negativ type og dimension mindst 2 må være enkeltsammenhængende.

Contents

Chapter 1

Introduction & Preliminaries

1.1 Introduction

The subject of this Ph.D.-thesis is somewhere in between discrete and continuous geometry, with the focus shifting from time to time. As always when working interdisciplinary the hope is to establish connections that can function as "bridges" and translate ideas from one field into the other.

The unifying concept is *distance* and in the discrete category we shall primarily be interested in *finite metric spaces*, but also more general distance spaces will be the subject of study. In the continuous setting we are interested in Riemannian manifolds and their generalizations in different directions into *semi-Riemannian spaces* and *length spaces*.

The "bridge" between the finite and the continuous setting is primarily to consider finite subsets of larger continuous spaces. One part of the project is concerned with abstracting from the concept of *ambient space*, thus refining a larger space to a finite subset. The question is how much of the geometry of a continuous space that is captured by such a refinement. And ultimately whether differential geometric concepts are preserved in some sense by a finite set, equipped with a refined structure such as e.g. a *distance function*.

This process opens the possibility of translating concepts from differential geometry into the framework of completely abstract finite spaces, where the geometry is described mainly by means of *linear algebra and combinatorics*. The geometry of finite spaces is tractable in a much more explicit way than for their continuous counterparts, and the finite setting opens up for e.g. *computer experimentation*, which may form the basis of new hypothesis with possible translations back to the continuous setting. This is something that will appear here and there throughout the thesis.

Translations of concepts from differential geometry to finite spaces could have interesting applications, also for "real life" problems. I must admit though, that the viewpoint in this thesis is not directed very much towards such applications.

In the other direction, the hope is that concepts from the geometry of finite sets will feed back on the continuous spaces via finite subsets of these. After all, finite spaces form a dense set in any reasonable topology on the category of (all interesting) continuous spaces!

Chapter 2 can be seen as an instance of the refinement process described above, while chapter 3 and especially chapter 4 can be seen as instances of the "feed back" process.

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Finally and most important, love goes to my wife Gitte, for always being supportive and indulgent. And thanks for making the great cover art!

An apology: From now on I will submit to the usual convention in mathematics and write in plural form, thus giving the reader a feeling that we are in this together...

1.2 Brief Summary of Contents

Here we shall give a summary of the most important content, section by section.

Chapter 2 Chapter 2 treats the geometry of finite subsets of the semi-Riemannian hyperquadrics $\mathbb{M}(n, \nu, \kappa)$, which include the simply connected Riemannian space forms.

In section 2.2 we introduce a distance with complex values on the semi-Riemannian hyperquadrics. This is just a natural extension of the usual Riemannian distance on the simply connected space forms to the semi-Riemannian cases. We establish a realizability result, Theorem 1, which gives conditions for when a finite distance space is realizable as a subset of $\mathbb{M}(n, \nu, \kappa)$. This is an extension of classical results of Menger, Schoenberg and Blumenthal.

The criterion for realizability of a finite distance space X in $\mathbb{M}(n, \nu, \kappa)$ is given in terms of the signature of a certain matrix $\mathbf{C}_\kappa(X)$, whose entries are a trigonometric function of distances in X. This matrix is the cornerstone of the theory. For a finite subset $X \subset \mathbb{M}(n, \nu, \kappa)$, $\mathbf{C}_\kappa(X)$ may be interpreted as a Gram matrix of a set of position vectors in an ambient semi-Euclidean space.

In section 2.3 we establish a formula, Theorem 2, that relates the determinant of the trigonometric $\mathbf{C}_\kappa(X)$-matrix to the geometry of a simplex X in $\mathbb{M}(n, \nu, \kappa)$. This is one of the most important results of the chapter, since it opens up interesting connections between the algebra of the $\mathbf{C}_\kappa(X)$-matrix and the geometry of simplices in $\mathbb{M}(n, \nu, \kappa)$.

In section 2.4 we pursue a $\mathbf{C}_\kappa$-matrix formulation of a duality studied in e.g. [24] and [29]. This can be stated as a duality between simplices, mapping spherical simplices to spherical simplices and hyperbolic simplices to simplices in a Lorentzian space form, the de Sitter-sphere. The duality interchange edge lengths and dihedral angles.

Hence we establish a formula for the dihedral angles of a simplex, Proposition 8, in terms of the $\mathbf{C}_\kappa(X)$-matrix of a simplex X. This formula establishes the *Gram matrix* *machinery*, or $\mathbf{C}_\kappa$-matrix theory, as a powerful tool to treat the geometry of simplices in high dimensional space forms. At the end of the section, we give some examples of this machinery: producing geometric relations from the algebra of the the $\mathbf{C}_\kappa$-matrix.

In section 2.5 we give an alternative formulation of the duality referred to above. This formulation, which is more global and intrinsic, is centered around half spaces and distance functions. The section is descriptive, and proofs are omitted. The conclusion of the discussion is, that the simply connected Riemannian space forms are isometric to subsets of measure spaces. This is important in connection with negative type, chapter 4.

This is not a new result, c.f. [27], but it seems important that it can be given a unified formulation for all curvatures, and that it can be seen as an instance of the duality as described for simplices.

Also, it turns out, in section 2.6, that the half space description of the duality for the Riemannian space forms has a counterpart for *weighted trees*, another class of metric spaces which will be of fundamental importance in this thesis. Essentially the same construction as for the space forms works for this class of metric spaces, with the same conclusion: *weighted trees are isometric to subsets of measure spaces.* This is also not a new result, but the formulation of it is new.

The final section of the chapter, section 2.7, collects some results and observations on the *isometric embedding problem*. The setup is to investigate the set of curvatures such that a given metric space is realizable in a space form with curvature in this set. Berestovskij has completed the analysis for metric spaces with 4 points, and shown that in these cases the set of *Riemannian embedding curvatures* form a interval, if nonempty. We give examples showing that the problem is much more complicated for larger spaces. But we also give an observation supporting that generically Berestovskij's result should hold, also for larger spaces.

Also we establish an interesting connection to the duality theory, described previously, via a concept called *complementary dual volume*: the measure of the set of oriented hyperplanes intersecting a given convex set.

Chapter 3 In Chapter 3 we apply the $\mathbf{C}_\kappa$-matrix theory to show the following central result:

Let X be a finite metric space. The following condition: "*there is a* $\kappa_0 < 0$ *such that* X *is realizable in a hyperbolic space of curvature* κ *for all* $\kappa < \kappa_0$", is satisfied if and only if X is a leaf space.

Here a *leaf space* consists of the set of degree 1 vertices of a finite weighted tree. The only if part is easy, and is already established in the framework of δ-hyperbolic spaces, c.f. [12]. However this part is also easily deduced from the matrix theory.

The constructive part is more difficult. In fact we are able to show a stronger result, Theorem 6. Here we find the limits, for $\kappa \to -\infty$, of the eigenvalues of the $\mathbf{C}_\kappa(X)$-matrix, when X is a weighted tree.

In the final section 3.2 we apply the theory developed to a discussion of the limiting geometry of an isometrically realized leaf space simplex as $\kappa \to -\infty$. We are able to find the limiting *altitudes* and *dihedral angles*. We end the chapter with a short discussion of relations to *ideal simplices* and the duality theory of chapter 2.

Chapter 4 In chapter 4 we discuss the concept of *negative type* of metric spaces. This is a classical concept, which has been applied in analysis and combinatorics, but is not a standard subject in Riemannian geometry. Riemannian manifolds of negative type include the simply connected space forms, and also complex hyperbolic spaces.

In section 4.1 we recapitulate some basic properties in connection with negative type. In section 4.2 we give a proof that the simply connected Riemannian space forms are of negative type, based on the duality discussion of chapter 2.

Section 4.3 is devoted to a measure theoretic formulation of negative type. We go into some detail here, since the feeling is that it is nonstandard material, at least from a Riemannian geometry perspective. In connection with the measure theoretic formulation we introduce the concept of *potential* of a distribution and several invariants, or *maximal energies*, related to a kernel (which could be the distance) on a metric space.

In section 4.4 we give some first applications of the theory developed. For example we give a simple argument that negative type of real and complex hyperbolic space implies strictly negative type of these spaces.

Section 4.5 is devoted to a discussion of the geometric significance of some of the concepts introduced. In particular we discuss the *extent* invariant, and show that the measure theoretic invariant introduced in section 4.3 corresponds to the extent as defined in [10]. We also discuss a relation between excess and extent for a compact metric space of negative type, Theorem 10.

In section 4.6 we use variation arguments to establish properties of potentials of maximal distributions. Theorem 12 is a reformulation of a theorem in [14], using the measure theoretic setup.

Then in section 4.7 we give some applications of the variational theory of section 4.6. First we discuss an application of the classical concept *subharmonicity* to distributions realizing the extent invariant. This applies to the distance kernel in spaces of nonpositive curvature.

The next subsection contains perhaps the most important application: a discussion of closed geodesics in compact length spaces of negative type. In particular it is shown that a compact Riemannian manifold of negative type and dimension at least 2 must be simply connected, Theorem 15, and also that points realizing the injectivity radius must be conjugate, Theorem 16.

Finally we have a subsection discussing maximal distributions and their potentials on the round sphere, the so far only known compact Riemannian manifold of negative type.

We conclude with a short subsection discussing possible constructions of Riemannian metrics of negative type and nonconstant curvature on the sphere.

1.3 Preliminaries & Definitions

In this section we will recapitulate some basic definitions and facts, and also introduce a few nonstandard concepts. Apart from concepts explicitly introduced we will feel free to use standard theory and terminology of differential and length space geometry.

Conventions on numbers

We use the convention $\mathbb{N}_0 := \{0, 1, 2, \ldots\} = \mathbb{N} \cup \{0\}$. And $\mathbb{R}_+ := [0, \infty)$, hence 0 is contained in $\mathbb{R}_+$. The invertible elements of $\mathbb{R}$ are denoted $\mathbb{R}^* := \mathbb{R} \setminus \{0\}$, and $\mathbb{R}^*_+ := \mathbb{R}_+ \cap \mathbb{R}^*$.

Fix a square root of -1 in $\mathbb{C}$, $\mathbf{i}^2 = -1$. For $x \in \mathbb{R}$, the convention $\sqrt{x} \in \mathbb{R}_+ \cup \mathbf{i}\mathbb{R}_+$ is used throughout. $\overline{z}$ will be used to denote the complex conjugate of $z \in \mathbb{C}$.

Distance Spaces

Since *distance* is the unifying concept in this thesis, the following deserves a definition:

Definition 1 (Metric Spaces). A metric on a set X is a function $d : X \times X \to \mathbb{R}$, such that for all $p, q, r \in X$:

1. $d(p, q) \geq 0$ (positivity)
2. $d(p, q) = 0$ if and only if $p = q$ (separation)
3. $d(p, q) = d(q, p)$ (symmetry)
4. $d(p, q) \leq d(p, r) + d(r, q)$ (triangle inequality)

A set with a metric is called a *metric space*. Generalizing things a bit, we define distance spaces:

Definition 2 (Distance Spaces). For $\mathcal{A} \subseteq \mathbb{C}$, an $\mathcal{A}$-distance on a set X is a function $d : X \times X \to \mathcal{A}$, such that for all $p, q \in X$:

1. $d(p, p) = 0$ (normalization)
2. $d(p, q) = d(q, p)$ (symmetry)

If (X, d) is a $\mathbb{R}_+$-distance space, then as usual we will introduce the diameter:

$$\operatorname{diam}(X) := \sup_{p,q \in X} \{d(p, q)\} \tag{1.1}$$

Notation 1. We will most of the time loosen the notation and just write X, whenever the specific appearance of the distance is not important. If X is a $\mathbb{C}$-distance space and $\lambda \in \mathbb{C}$ a scalar, then λX means the distance space with distance function λd.

Definition 3 (Isometries). If (X, d_X) and (Y, d_Y) are distance spaces and there is a map $\phi : X \to Y$ such that $d_X(p, q) = d_Y(\phi(p), \phi(q)),\ \forall p, q \in X$, we say that X is realizable in Y and write $X \overset{isom}{\hookrightarrow} Y$. ϕ is called a *realization* or an *isometry*.

(X, d_X) and (Y, d_Y) are *isometric*, $X \underset{isom}{\cong} Y$, if there is a bijective realization $X \overset{isom}{\hookrightarrow} Y$.

Note that a realization $\phi : X \to Y$ is not necessarily injective, unless the following property is satisfied:

Definition 4 (Separation Axiom). A distance space (X, d) is said to satisfy the *separation axiom* if

$$p \neq q \text{ and } d(p, q) = 0 \implies \exists r \in X : d(p, r) \neq d(q, r)$$

Antipodality & Excess

Definition 5 (Antipodality). Let X be a $\mathbb{C}$-distance space with $|X| > 2$. $p, q \in X$ are defined to be antipodal in X iff for all $r \in X$:

$$d(p, r) + d(r, q) = d(p, q) \tag{1.2}$$

An easy argument shows:

Observation 1. If $p, q \in X$ are antipodal in (X, d) and d is a metric then $\operatorname{diam}(X) = d(p, q)$

Definition 6. Let (X, d) be a $\mathbb{C}$-distance space. For $p, q, r \in X$ define the excess function:

$$e_{p,q}(r) = d(p, r) + d(r, q) - d(p, q) \tag{1.3}$$

For r fixed, $e_{p,q}(r)$ is symmetric in p, q by the symmetry requirement of a distance space. Clearly $e_{p,q}(r) = 0$ for all $r \in X$ iff p, q are antipodal.

Definition 7. Let (X, d) be a $\mathbb{R}_+$-distance space with $\operatorname{diam}(X) < \infty$. Define:

$$\operatorname{exc}(X) := \inf_{p,q \in X} \{\sup_{r \in X}\{e_{p,q}(r)\}\} \tag{1.4}$$

An $\mathbb{R}_+$-distance space is a metric space iff $e_{p,q}$ is a nonnegative function for all p, q. So for a metric space we always have $\operatorname{exc}(X) \geq 0$. We also see that if X has a pair of antipodal points then $\operatorname{exc}(X) = 0$. The converse also holds when (X, d) is compact, since then the inf's and sup's are realized by continuity.

Observation 2. For a compact metric space $\operatorname{exc}(X) = 0$ iff X has a pair of antipodal points.

Trigonometric functions

For κ and x in R we will define

$$\mathbf{c}_\kappa(x) := \begin{cases} \cos(\sqrt{\kappa}x) & \text{for } \kappa \neq 0 \\ 1 - \frac{x^2}{2} & \text{for } \kappa = 0 \end{cases} \tag{1.5}$$

$$\mathbf{s}_\kappa(x) := \begin{cases} \sin(\sqrt{\kappa}x) & \text{for } \kappa \neq 0 \\ x & \text{for } \kappa = 0 \end{cases} \tag{1.6}$$

Note that for $z \in \mathbb{C}:\ \cos(\mathbf{i}z) = \cosh(z)$, while $\sin(\mathbf{i}z) = \mathbf{i}\sinh(z)$. With the trigonometric functions we shall associate subsets of $\mathbb{C}$:

Definition 8. For $\kappa \in \mathbb{R}$ define the subset $\mathbb{C}_\kappa \subset \mathbb{C}$ as:

$$\mathbb{C}_\kappa := \begin{cases} \{z \in \mathbb{C} \,|\, \mathbf{c}_\kappa(z) \in \mathbb{R}, 0 \le \Re(z) \le \frac{\pi}{\sqrt{\kappa}},\ \Im(z) \ge 0\} & \text{for } \kappa > 0 \\ \{z \in \mathbb{C} \,|\, \mathbf{c}_\kappa(z) \in \mathbb{R}, \Re(z) \ge 0,\ \Im(z) \ge 0\} & \text{for } \kappa = 0 \\ \{z \in \mathbb{C} \,|\, \mathbf{c}_\kappa(z) \in \mathbb{R}, \Re(z) \ge 0\,, 0 \le \Im(z) \le \frac{\pi}{\sqrt{|\kappa|}}\} & \text{for } \kappa < 0 \end{cases} \tag{1.7}$$

Another characterization is:

$$\begin{aligned} \mathbb{C}_\kappa &= [0, \tfrac{\pi}{\sqrt{\kappa}}] \cup \mathbf{i}\mathbb{R}_+ \cup (\tfrac{\pi}{\sqrt{\kappa}} + \mathbf{i}\mathbb{R}_+) \text{ for } \kappa > 0 \\ \mathbb{C}_0 &= \mathbb{R}_+ \cup \mathbf{i}\mathbb{R}_+ \\ \mathbb{C}_\kappa &= \mathbf{i}\overline{\mathbb{C}_{|\kappa|}} \text{ for } \kappa < 0 \end{aligned}$$

Remark 1. $\mathbb{C}_\kappa \subset \mathbb{C}$ is defined such that it is the set of values for a distance defined on the semi-Riemannian space forms $\mathbb{M}(n, \nu, \kappa)$. See chapter 2.

Matrix conventions

The set of $m \times n$-matrices with entries in a subset $\mathcal{A} \subseteq \mathbb{C}$ are denoted $\mathrm{M}_{m,n}(\mathcal{A})$, and $\mathrm{M}_n(\mathcal{A})$ in the square case. The subset of symmetric, $n \times n$ matrices is written $\mathrm{Sym}_n(\mathcal{A}) := \{\mathbf{X} \in \mathrm{M}_n(\mathcal{A}) |\, \mathbf{X} = \mathbf{X}^t\}$. $\mathrm{Gl}_n(\mathbb{R})$ denotes the invertible matrices with real entries. To specify the entries of a matrix the notation $\mathbf{X} = [x_{ij}]$ is used.

A finite $\mathcal{A}$-distance space $X = \{p_1, \ldots, p_n\}$ is completely characterized by its $n \times n$-distance matrix $\mathbf{D}_X = [d_{ij}]$, where $d_{ij} := d(p_i, p_j)$. $\mathcal{D}_n(\mathcal{A})$ will denote the set of all $n \times n$ $\mathcal{A}$-distance matrices:

$$\mathcal{D}_n := \{[d_{ij}] \in \mathrm{Sym}_n(\mathcal{A}) | d_{ii} = 0, \forall i\}$$

The *signature* of a matrix $\mathbf{X} \in \mathrm{Sym}_n(\mathbb{R})$ is the triple (n_-, n_+, n_0), where n_- is the number of negative eigenvalues, also called the *index*, n_+ is the number of positive eigenvalues and n_0 is the number of negative eigenvalues. The notation $\iota(\mathbf{X})$ and $\rho(\mathbf{X})$ will also be used to denote respectively the index and the number of positive eigenvalues.

$\det(\mathbf{X})$ is the determinant of $\mathbf{X}$. Sometimes the notation $|\mathbf{X}|$ will be used for the determinant in order to save space. $|\cdot|$ will also be used to denote the cardinality of a set and the absolute value of a complex number; the meaning should be clear from context.

Recall that the *cofactor* matrix $\mathrm{cof}(\mathbf{X}) = [c_{ij}]$ of a square matrix $\mathbf{X}$ is the matrix of signed minors defined as $c_{ij} := (-1)^{i+j}|\mathbf{X}^i_j|$, where $\mathbf{X}^i_j$ is the submatrix obtained by deleting column i and row j. It satisfies

$$\mathbf{X}\,\mathrm{cof}(\mathbf{X}) = \mathrm{cof}(\mathbf{X})\mathbf{X} = \det(\mathbf{X})\mathbf{I}$$

The following formula (for a symmetric matrix $\mathbf{X}$), will prove useful:

$$|\mathbf{X}||\mathbf{X}_{ij}| = |\mathbf{X}_i||\mathbf{X}_j| - |\mathbf{X}^i_j|^2 \tag{1.8}$$

Here $\mathbf{X}_i$ is the principal submatrix of $\mathbf{X}$ obtained by deleting row and column i, while $\mathbf{X}_{ij}$ is obtained by deleting rows and columns i, j, etc. Note that $|\mathbf{X}_i| = c_{ii}$.

$\mathbf{C}_\kappa$-matrices

The following matrix will play a fundamental role throughout this thesis:

Definition 9. Let X be a finite $\mathbb{C}$-distance space with n points and distance matrix $\mathbf{D}_X = [d_{ij}] \in \mathcal{D}_n(\mathbb{C})$.

- For $\kappa \in \mathbb{R} \setminus \{0\}$ define the $n \times n$ matrix $\mathbf{C}_\kappa(X) := [\mathbf{c}_\kappa(d_{ij})]$.
- For $\kappa = 0$ define the $(n+1) \times (n+1)$ matrix:

$$\mathbf{C}_0(X) := \begin{pmatrix} 0 & -1 & -1 & \cdots & -1 \\ 1 & 1 & 1 - \frac{d_{1,2}^2}{2} & \cdots & 1 - \frac{d_{1,n}^2}{2} \\ 1 & 1 - \frac{d_{2,1}^2}{2} & 1 & \cdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 1 - \frac{d_{n-1,n}^2}{2} \\ 1 & 1 - \frac{d_{n,1}^2}{2} & \cdots & 1 - \frac{d_{n,n-1}^2}{2} & 1 \end{pmatrix} \tag{1.9}$$

  We will use the convention that the rows and columns of $\mathbf{C}_0(X)$ are indexed by $\{0, 1, \ldots, n\}$.

Note that taking principal submatrices of $\mathbf{C}_\kappa(X)$ corresponds to "deleting" points of X.

Cayley-Menger matrix The classical Cayley-Menger matrix of X is defined as follows: Extend X with a “virtual” point p_0 s.t. $d(p_0, p_i) = 1$ for $i > 0$. Then the Cayley-Menger matrix $\mathbf{CM}(X) \in \mathrm{Sym}_{n+1}(\mathbb{R})$ has entries $[d_{ij}^2]$ for $i, j \in \{0, 1, \ldots, n\}$. $\mathbf{CM}(X)$ can be obtained from $\mathbf{C}_0(X)$ by elementary row and column operations.

For various reasons the choice of "normalization" in $\mathbf{C}_0(X)$ fits slightly better into the general framework than $\mathbf{CM}(X)$. One indication of this is the following which is not difficult to show:

$$\det(\mathbf{C}_\kappa(X)) = \det(\mathbf{C}_0(X))\kappa^{n-1} + \text{higher order terms} \qquad \text{(Analytic Structure)}$$

Note that even though $\mathbf{C}_0(X)$ is not symmetric (1.8) remains valid, when we for the indices have $i, j \geq 1$.

We have the following formula for the determinant of a $\mathbb{C}$-distance space on 3-points, which we choose to call *Heron's Formula* because of its relation to a classical formula:

Lemma 1 (Heron's Formula). *Let $X = \{p_1, p_2, p_3\}$ be a $\mathbb{C}$-distance space, with distances: $d(p_1, p_2) = a$, $d(p_2, p_3) = b$, $d(p_3, p_1) = c$ and put $s = \frac{1}{2}(a + b + c)$. Then:*

$$\det(\mathbf{C}_\kappa(X)) = 4\,\mathbf{s}_\kappa(s)\mathbf{s}_\kappa(s-a)\mathbf{s}_\kappa(s-b)\mathbf{s}_\kappa(s-c) \tag{1.10}$$

Proof. Simply expand the determinant and apply the usual identities for $\mathbf{c}_\kappa$ and $\mathbf{s}_\kappa$. □

From Heron's Formula it is easy to deduce:

Lemma 2. *Let (X, d) be a $\mathbb{C}_\kappa$-distance space:*

- *For $Y = \{p_1, p_2, p_3\}$ we have $\det(\mathbf{C}_\kappa(Y)) = 0$ iff $s = \frac{\pi}{\sqrt{\kappa}}$, or one point is in "between" the two others, i.e. one of the three excesses vanish.*

- *X satisfies the separation axiom, Definition 4, iff: for every pair of distinct points with $d(p_1, p_2) = 0$ there is a point $p_3 \in X$ such that $\det(\mathbf{C}_\kappa(Y)) \neq 0$, where $Y = \{p_1, p_2, p_3\}$.*

This means that when the distances are in $\mathbb{C}_\kappa$, $\mathbf{C}_\kappa(Y)$ is singular iff two of the three points are indistinguishable, one points is in between the two others, or the *circumference* is $2s = \frac{2\pi}{\sqrt{\kappa}}$; this means that Y is realizable in $\frac{1}{\sqrt{\kappa}}\mathbb{S}^1$ (which is either $\mathbb{M}(1, 0, |\kappa|)$ or $\mathbb{M}(1, 1, -|\kappa|)$ see chapter 2).

Semi-Euclidean spaces and Gram matrices

If $(V, \langle\cdot,\cdot\rangle)$ is a $\mathbb{R}$-vector space with a symmetric, bilinear form, the *Gram-matrix* of a finite set of vectors $X = \{v_1, \ldots, v_m\} \in V$ is the matrix

$$\mathbf{G}_X = [\langle v_i, v_j\rangle] \in \mathrm{Sym}_m(\mathbb{R}) \tag{1.11}$$

One formulation of a fundamental property is:

Proposition 1 (Sylvester's Law of Inertia). *Let $(V, \langle\cdot,\cdot\rangle)$ be a finite dimensional $\mathbb{R}$-vector space with a symmetric, $\mathbb{R}$-bilinear form, and let $X = \{v_1, \ldots, v_n\}$ be a basis for V.*

1. *The signature* (n_-, n_+, n_0) *of the Gram-matrix* $\mathbf{G}_X$ *is independent of the basis* X.

2. *For any finite subset* $Y \subset V : \iota(\mathbf{G}_Y) \leq n_-$, $\rho(\mathbf{G}_Y) \leq n_+$ *and if* Y *is a linearly dependent set, then* $\mathbf{G}_Y$ *is singular.*

For $n, \nu \in \mathbb{N}_0$, with $\nu \leq n$, $\mathbb{R}^n_\nu$ will denote the *semi-Euclidean* space of dimension n and index ν, i.e. the scalar product is:

$$\langle x, y \rangle = -\sum_{i=1}^{\nu} x_i y_i + \sum_{i=\nu+1}^{n} x_i y_i, \tag{1.12}$$

where the x_i's and the y_i's are the coordinates of x, y with respect to the standard basis. A linear subspace $V \subseteq \mathbb{R}^n_\nu$ is called *nondegenerate* if $\langle \cdot, \cdot \rangle$ restricted to V is nondegenerate, which means that the Gram matrix for a basis X for V is regular:

$$\det(\mathbf{G}_X) \neq 0, \tag{1.13}$$

or equivalently that $\operatorname{rank}(\mathbf{G}_Y) = \dim(V)$, whenever a finite set of vectors Y span V.

Let $\mathbf{I}_\nu$ be the Gram-matrix of the standard basis in $\mathbb{R}^n_\nu$:

$$\mathbf{I}_\nu = \operatorname{diag}(\underbrace{-1, \ldots, -1}_{\nu \text{ times}}, \underbrace{1, \ldots, 1}_{n-\nu \text{ times}}) \tag{1.14}$$

The Gram matrix for a set $X = \{v_1, \ldots, v_m\} \subset \mathbb{R}^n_\nu$ of m vectors can also be written $\mathbf{G}_X = \mathbf{X}^t \mathbf{I}_\nu \mathbf{X}$, where $\mathbf{X} \in \mathrm{M}_{n,m}(\mathbb{R})$ is the matrix whose i'th column is (the coordinates of) v_i.

Any matrix in $\mathrm{Sym}_m(\mathbb{R})$ may be interpreted as the Gram-matrix of a set of m vectors in some $\mathbb{R}^n_\nu$: For $\mathbf{G} \in \mathrm{Sym}_m(\mathbb{R})$ there is an invertible matrix $\mathbf{Y} \in \mathrm{Gl}_m(\mathbb{R})$, s.t.:

$$\mathbf{Y}^t \mathbf{G} \mathbf{Y} = \mathbf{I}(n_-, n_+, n_0), \tag{1.15}$$

where $\mathbf{I}(n_-, n_+, n_0)$ is the *standard diagonal matrix of signature* (n_-, n_+, n_0),

$$\mathbf{I}(n_-, n_+, n_0) = \operatorname{diag}(\underbrace{-1, \ldots, -1}_{n_- \text{ times}}, \underbrace{1, \ldots, 1}_{n_+ \text{ times}}, \underbrace{0, \ldots, 0}_{n_0 \text{ times}}) \tag{1.16}$$

Then:

$$\mathbf{G} = (\mathbf{Y}^{-1})^t \mathbf{I}(n_-, n_+, n_0) \mathbf{Y}^{-1} \tag{1.17}$$

Hence defining $\mathbf{X} \in \mathrm{M}_{m-n_0,m}(\mathbb{R})$ to be the matrix obtained from $\mathbf{Y}^{-1}$ be deleting the last n_0 rows, $\mathbf{G}$ is the Gram-matrix for the set of columns of $\mathbf{X}$ considered as vectors in $\mathbb{R}^{m-n_0}_{n_-}$.

Remark 2. Note that when $\mathbf{G}$ is singular, there is no guarantee that the vectors obtained by the procedure above, i.e. the columns of $\mathbf{X}$, are *distinct*.

Chapter 2

Geometry of Finite Sets in Space Forms

In this chapter we shall study the geometry of semi-Riemannian manifolds of constant curvature, with a special focus on finite subsets of these. For fundamentals of semi-Riemannian geometry, refer to [21].

This chapter is mainly a reformulation and generalization of the material in [18]. The main message is that the geometry of finite subsets of semi-Riemannian hyperquadrics, which include the usual simply connected Riemannian space forms, can be treated in a unified way. The approach is via Gram matrices of position vectors in an ambient semi-Euclidean space. But defining a distance (with complex values), extending the usual definition of the Riemannian distance to the indefinite spaces, the Gram matrix of a finite subset X can also be viewed from a more "intrinsic angle" as the trigonometric $\mathbf{C}_\kappa$-matrix of the distance space X.

This is in the spirit of the classic book [2], where the theory is developed for spheres, real projective spaces and hyperbolic spaces, from an intrinsic viewpoint.

2.1 Geometry of Hyperquadrics

This first section will be a repetition of some standard facts and terminology. Recall that the *index* of a semi-Riemannian manifold (M, g) is the index of (a matrix for) the metric tensor g. As for matrices we shall use the notation $\iota(M)$ to denote the index.

Models for those semi-Riemannian space forms we shall study are provided by *hyperquadrics* in semi-Euclidean spaces:

Definition 10. For $\kappa \in \mathbb{R}$ and $n, \nu \in \mathbb{N}_0$ with $\nu \leq n$ define $\mathbb{M}(n, \nu, \kappa)$ as:

- If $\nu = 0$ and $\kappa < 0$: $\mathbb{M}(n, 0, \kappa) := \{x \in \mathbb{R}^{n+1}_1 \,|\, \langle x, x \rangle = \frac{1}{\kappa}, x_1 > 0\}$

- If $\nu = n$ and $\kappa > 0$: $\mathbb{M}(n, n, \kappa) := \{x \in \mathbb{R}^{n+1}_n \,|\, \langle x, x \rangle = \frac{1}{\kappa}, x_{n+1} > 0\}$

- And otherwise

$$\mathbb{M}(n,\nu,\kappa) := \begin{cases} \{x \in \mathbb{R}^{n+1}_{\nu} \mid \langle x, x\rangle = \frac{1}{\kappa}\} & \text{for } \kappa > 0 \\ \mathbb{R}^{n}_{\nu} & \text{for } \kappa = 0 \\ \{x \in \mathbb{R}^{n+1}_{\nu+1} \mid \langle x, x\rangle = \frac{1}{\kappa}\} & \text{for } \kappa < 0 \end{cases} \tag{2.1}$$

In every case $\mathbb{M}(n,\nu,\kappa)$ is equipped with the metric tensor inherited from the ambient space, and is an orientable, connected, semi-Riemannian manifold of dimension n, index ν and constant curvature κ if $n \geq 2$.

By $\mathbb{M}(n,\nu,0) := \mathbb{R}^n_\nu$, we mean $\mathbb{R}^n_\nu$ regarded as an *affine* manifold, while whenever we talk about an *ambient* semi-Euclidean space $\mathbb{R}^{n+1}_\nu$, we consider this as a *linear* space.

Remark 3. Sometimes it is useful to think of the affine $\mathbb{M}(n,\nu,0)$ as an affine hypersurface of an *ambient* $\mathbb{R}^{n+1}_{\nu_0}$. Then many arguments does not require special attention in the otherwise exceptional case $\kappa = 0$.

The topology is:

$$\mathbb{M}(n,\nu,\kappa) \underset{homeo}{\sim} \begin{cases} \mathbb{S}^{n-\nu} \times \mathbb{R}^{\nu} & \text{for } \kappa > 0 \\ \mathbb{S}^{\nu} \times \mathbb{R}^{n-\nu} & \text{for } \kappa < 0, \end{cases} \tag{2.2}$$

or a connected component of the above, when the product contains a $\mathbb{S}^0$-factor.

Remark 4. Unlike [21], we use $\mathbb{M}(n,\nu,\kappa)$ to denote the semi-Riemannian hyperquadrics even in the cases when these are *not simply connected*. This is the case when $\mathbb{M}(n,\nu,\kappa)$ contains a $\mathbb{S}^1$ factor, i.e. for $n-\nu = 1, \kappa > 0$ and for $\nu = 1, \kappa < 0$.

In the Riemannian cases, $\nu = 0$, we shall write $\mathbb{M}(n,\kappa) := \mathbb{M}(n,0,\kappa)$, and sometimes more specifically $\mathbb{S}(n,\kappa)$ for the spheres, $\kappa > 0$, and $\mathbb{H}(n,\kappa)$ for the hyperbolic spaces, $\kappa < 0$.

Consider a geodesic triangle with side lengths a, b, c and opposite angles A, B, C in one of the Riemannian space forms $\mathbb{M}(n,\kappa)$. With the definition of the trigonometric functions, (1.5) (1.6), the *sine relation* becomes:

$$\frac{\mathbf{s}_\kappa(a)}{\sin(A)} = \frac{\mathbf{s}_\kappa(b)}{\sin(B)} = \frac{\mathbf{s}_\kappa(c)}{\sin(C)}, \tag{2.3}$$

And for $\kappa \neq 0$ the *cosine relation* is:

$$\mathbf{c}_\kappa(c) = \mathbf{c}_\kappa(a)\mathbf{c}_\kappa(b) + \mathbf{s}_\kappa(a)\mathbf{s}_\kappa(b)\cos(C) \tag{2.4}$$

Causal character The usual conventions regarding *causal character* of vectors and geodesics etc. are used. A tangent vector $v \in T_pM$ of a semi-Riemannian manifold $(M, \langle\cdot,\cdot\rangle)$ is called

- spacelike if $\langle v, v\rangle > 0$ or $v = 0$
- lightlike if $\langle v, v\rangle = 0$ and $v \neq 0$
- timelike if $\langle v, v\rangle < 0$

Notation 2 (Tilde-notation). For $\kappa \neq 0$ and a geometric object in $\mathbb{M} = \mathbb{M}(n, \nu, \kappa)$, e.g. a subspace $S \subset \mathbb{M}(n, \nu, \kappa)$, we will use a tilde to denote the object in the ambient space that corresponds to the object in $\mathbb{M}$ by intersection, i.e. $S = \tilde{S} \cap \mathbb{M}$. Hence for a point $p \in \mathbb{M}$, $\tilde{p}$ will be used to denote its position vector in $\mathbb{R}^{n+1}_{\nu_0}$ (where $\nu_0 = \nu$ for $\kappa > 0$ and $\nu_0 = \nu + 1$ for $\kappa < 0$). This notation is also used for maps, e.g. ϕ is the *restriction* of $\tilde{\phi}$ to $\mathbb{M}$.

Geodesics Every geodesic of $\mathbb{M}(n, \nu, \kappa)$ is complete, i.e. defined on all of $\mathbb{R}$, and is either smoothly closed or injective, and defines a one dimensional subspace. For $\kappa > 0$ spacelike geodesics γ are closed with period $\frac{2\pi}{\sqrt{\kappa}}$ and images $\gamma(\mathbb{R})$ isometric to $\mathbb{S}(1, \kappa)$. Lightlike and timelike geodesics are injective with images homeomorphic to $\mathbb{R}$, hence timelike geodesics are isometric to $\mathbb{R}^1_1 = \mathbb{M}(1, 1, 0)$. For $\kappa < 0$ the properties of spacelike and timelike geodesics are reversed; timelike geodesics are closed with period $\frac{2\pi}{\sqrt{|\kappa|}}$ and spacelike geodesics are isometric to $\mathbb{R}^1_0 = \mathbb{M}(1, 0, 0)$.

For $\kappa \neq 0$, the image of a geodesic $\gamma(\mathbb{R})$ is exactly a connected component of the intersection of $\mathbb{M}(n, \nu, \kappa)$ with a 2-dimensional linear subspace of the ambient $\mathbb{R}^{n+1}_{\nu_0}$. The image of any lightlike geodesic γ is a connected component of the intersection with a degenerate plane $\tilde{P} \subset \mathbb{R}^{n+1}_{\nu_0}$. Such a component, γ, is also a lightlike geodesic, $\tilde{\gamma}$, of the ambient space.The intersection $\tilde{P} \cap \mathbb{M}(n, \nu, \kappa)$ has exactly two connected components (see [21] 4.28), hence every lightlike geodesic has an "opposite" lightlike geodesic.

For $\kappa = 0$ every geodesic is injective; the (images of) geodesics are exactly the 1-dimensional affine subspaces of $\mathbb{R}^n_\nu$.

For $\kappa \neq 0$ and two distinct points $p, q \in \mathbb{M}(n, \nu, \kappa)$, the following situations can occur, cf. [21] p. 149:

1. p, q lie on a unique geodesic, which is either periodic or one to one.
2. p, q lie on a periodic geodesic γ with $\gamma(0) = p$ and $\gamma(\frac{\pi}{\sqrt{|\kappa|}}) = q$.
3. p, q are not joined by any geodesic.

In case 2 we say that p, q are *antipodal* in $\mathbb{M}(n, \nu, \kappa)$. We shall see shortly, that this notion of antipodality corresponds to the one given in Definition 5. Antipodal points are precisely points with position vectors such that: $\tilde{p} = -\tilde{q}$ in the ambient semi-Euclidean space. Antipodal points are connected by infinitely many periodic geodesics if $n > 1$, all of which are spacelike if $\kappa > 0$ and timelike if $\kappa < 0$.

If there is a geodesic joining p, q, the points are called geodesically connected. A subset $X \subseteq \mathbb{M}(n, \nu, \kappa)$ is called geodesically connected if any two points in X are geodesically connected.

For $\kappa = 0$ every pair of points $p, q \in \mathbb{R}^n_q$ are joined by a unique geodesic.

Terminology 1 (Convexity). In the Riemannian cases we shall often use the notion of convex subsets . In the simple context of the space forms $\mathbb{M}(n, \kappa)$, we will use the following definitions: A subset $C \subseteq \mathbb{M}(n, \kappa)$ is called convex if any two points $p, q \in C$ are joined by a *unique* geodesic γ, which is minimal in $\mathbb{M}(n, \kappa)$ and lies entirely in C.

Hence a (small) geodesic segment and an open hemisphere of $\mathbb{S}(n, \kappa)$ are convex, while $\mathbb{S}(n, \kappa)$ and a closed hemisphere are not.

For $\kappa \leq 0$ the convex hull of a subset X is the minimal convex set $C \subseteq \mathbb{M}(n, \kappa)$ containing X. For $\kappa > 0$ and X contained in an open hemisphere, we use the same definition of the convex hull, while if X is *not contained* in an open hemisphere, the convex hull is defined to be the entire sphere $\mathbb{M}(n, \kappa)$. We will use $\Delta(X)$ to denote the convex hull of a subset $X \subseteq \mathbb{M}(n, \kappa)$.

The notions of convex sets and convex hull easily generalizes to the semi-Riemannian and nonconstant curvature cases. This will not be needed here…

2.2 Distance in $\mathbb{M}(n, \nu, \kappa)$

The geometry of $\mathbb{M}(n, \nu, \kappa)$ can be treated from the perspective of the ambient semi-Euclidean space. But the main interest here is *distances* and the viewpoint will be mostly *intrinsic*. One partial goal is to abstract from the concept of "ambient space", thus refining properties of the continuous space to properties of a finite distance space. Schematically the refinement goes:

semi-Euclidean space→semi-Riemannian space forms→discrete distance spaces

However when it makes life easier (which is quite often!), we will feel free to use the machinery of the ambient space.

In the spirit of [29] and [30], but slightly different, we shall introduce a *complex distance* on $\mathbb{M}(n, \nu, \kappa)$.

Definition 11. For $\kappa \neq 0$ and $p, q \in \mathbb{M}(n, \nu, \kappa)$, let $d_{\mathbb{C}}(p, q)$ be the unique complex number in $\mathbb{C}_\kappa$ such that:

$$\mathbf{c}_\kappa(d_{\mathbb{C}}(p, q)) = \frac{\langle \tilde{p}, \tilde{q} \rangle}{\sqrt{\langle \tilde{p}, \tilde{p} \rangle}\sqrt{\langle \tilde{q}, \tilde{q} \rangle}} = \kappa \langle \tilde{p}, \tilde{q} \rangle, \tag{2.5}$$

where $\langle\cdot,\cdot\rangle$ denotes the scalar product of the ambient space. For $\kappa = 0$ and $p, q \in \mathbb{R}^n_\nu$, let $d_{\mathbb{C}}(p,q)$ be the unique complex number in $\mathbb{C}_0$ such that:

$$d_{\mathbb{C}}(p,q)^2 = \langle p-q, p-q\rangle = \langle p,p\rangle + \langle q,q\rangle - 2\langle p,q\rangle \tag{2.6}$$

In the Riemannian cases, $\nu = 0$, $d_{\mathbb{C}}$ coincides with the usual definition/formula for the Riemannian distance on $\mathbb{R}^n$ and, for $\kappa \neq 0$, on the hyperquadric models $\mathbb{M}(n,\kappa)$. So it is only in the cases $\nu > 0$ we obtain anything non standard. The following couple of pages summarize some basic properties of this complex distance[1]. Most of these follow easily from the description of the geometry of hyperquadrics given in [21].

Remark 5. If $X \subset \mathbb{M}(n,\nu,\kappa)$ and $\kappa \neq 0$, then simply by definition of $d_{\mathbb{C}}$ and $\mathbf{C}_\kappa(X)$, Definition 9, we have:

$$\mathbf{C}_\kappa(X) = \kappa \mathbf{G}_{\tilde{X}} = \kappa[\langle \tilde{p}_i, \tilde{p}_j\rangle], \tag{2.7}$$

where $\tilde{X}$ is the set of position vectors in the ambient space. For $\kappa = 0$ we shall see in the proof of Theorem 1 below, that also $\mathbf{C}_0(X)$ is closely related to a Gram matrix.

We immediately have:

Proposition 2. *$d_{\mathbb{C}}$ is symmetric and $d_{\mathbb{C}}(p,p) = 0$ for all $p \in \mathbb{M}(n,\nu,\kappa)$. Hence $d_{\mathbb{C}}$ is a $\mathbb{C}_\kappa$-distance on $\mathbb{M}(n,\nu,\kappa)$. Furthermore*

$$\left(\mathbb{M}(n,\nu,\kappa), \mathbf{i}\overline{d_{\mathbb{C}}}\right) \underset{isom}{\cong} \left(\mathbb{M}(n, n-\nu, -\kappa), d_{\mathbb{C}}\right) \tag{2.8}$$

Proof. The first statement is obvious. For the other, multiply the scalar product in $\mathbb{R}^{n+1}_{\nu_0}$ by -1. This corresponds to multiplying the metric tensor on $T\mathbb{M}$ by -1; then curvature and causal character is reversed. $\square$

Proposition 38 in [21] (p. 149) translates directly into a distance statement, which remains valid for $\kappa = 0$:

Proposition 3. *Let $p, q \in \mathbb{M}(n,\nu,\kappa)$ be distinct nonantipodal points, and put*

$$r_1 := \sup_{z\in\mathbb{C}_\kappa}\{\Re(z)\},\ r_2 := \sup_{z\in\mathbb{C}_\kappa}\{\Im(z)\},$$

1. *If $d_{\mathbb{C}}(p,q) \in (0, r_1)$, then p, q lie on a unique spacelike geodesic.*

2. *If $d_{\mathbb{C}}(p,q) = 0$, then p, q lie on a unique lightlike geodesic.*

3. *If $d_{\mathbb{C}}(p,q) \in \mathbf{i}(0, r_2)$, then p, q lie on a unique timelike geodesic.*

And otherwise p and q are not geodesically connected.

---

[1] Hopefully, by the end of this chapter the (patient) reader should be convinced that the extension of $d_{\mathbb{C}}$ to the semi-Riemannian cases is in fact quite useful!

For $\kappa \neq 0$ points that are not geodesically connected either have distance $\frac{\pi}{\sqrt{\kappa}}$ or distance in $\mathbb{C}_\kappa \setminus \mathbb{R}_+ \cup \mathbf{i}\mathbb{R}_+$. The following clarifies what it means geometrically to have distance $\frac{\pi}{\sqrt{\kappa}}$:

Lemma 3. *Assume $\kappa \neq 0$. If $d_{\mathbb{C}}(p,q) = \frac{\pi}{\sqrt{\kappa}}$ then either $\tilde{p} = -\tilde{q}$ or the plane* $\operatorname{span}(\tilde{p},\tilde{q}) \subset \mathbb{R}^{n+1}_{\nu_0}$ *is degenerate and intersects $\mathbb{M}(n,\nu,\kappa)$ in two lightlike geodesics γ_1, γ_2 with $d_{\mathbb{C}}(\gamma_1(t), \gamma_2(s)) = \frac{\pi}{\sqrt{\kappa}}$ for all $t, s \in \mathbb{R}$.*

Proof. $d_{\mathbb{C}}(p,q) = \frac{\pi}{\sqrt{\kappa}}$ means that $\kappa\langle\tilde{p},\tilde{q}\rangle = \mathbf{c}_\kappa(\frac{\pi}{\sqrt{\kappa}}) = -1$. But then $\mathbf{C}_\kappa(\{p,q\}) = \kappa\mathbf{G}_{\{\tilde{p},\tilde{q}\}}$ is clearly singular. This means that either $\tilde{p},\tilde{q}$ are linearly dependent, hence $\tilde{p} = -\tilde{q}$, or $\operatorname{span}(\tilde{p},\tilde{q})$ is degenerate (see the introduction).

For a proof that the degenerate plane intersects $\mathbb{M}$ in two disjoint lightlike geodesics, see [21], Prop. 4.28. Any two points on these geodesics lies in the same degenerate plane. Hence $\det(\mathbf{C}_\kappa(Y)) = 0$, when $Y = \{r,s\}$ consists of two such points. But this is only possible if $\mathbf{c}_\kappa(d_{\mathbb{C}}(r,s)) = \pm 1$, i.e. $d_{\mathbb{C}}(r,s) = 0$ (r, s are on the same geodesic) or $d_{\mathbb{C}}(r,s) = \frac{\pi}{\sqrt{\kappa}}$ (r, s are on different geodesics). □

Let's make it clear that antipodality in $\mathbb{M}(n,\nu,\kappa)$, in the sense that $\tilde{p} = -\tilde{q}$, implies antipodality in the sense of Definition 5:

Lemma 4. *If $\kappa \neq 0$ and $p, q \in \mathbb{M}(n,\nu,\kappa)$ are antipodal in the sense that $\sigma_A(p) = q$, where σ_A is the antipodal isometry $\tilde{\sigma}_A : \tilde{p} \mapsto -\tilde{p}$, then for any $X \subseteq \mathbb{M}(n,\nu,\kappa)$ with $\{p,q\} \subseteq X$, p and q are antipodal in X according to Definition 5.*

Proof. Note that for any finite set X containing $\{p,q\}$, the position vectors are linearly dependent, hence $\mathbf{C}_\kappa(X) = \kappa\mathbf{G}_{\tilde{X}}$ is singular. The result then follows from Lemma 2. □

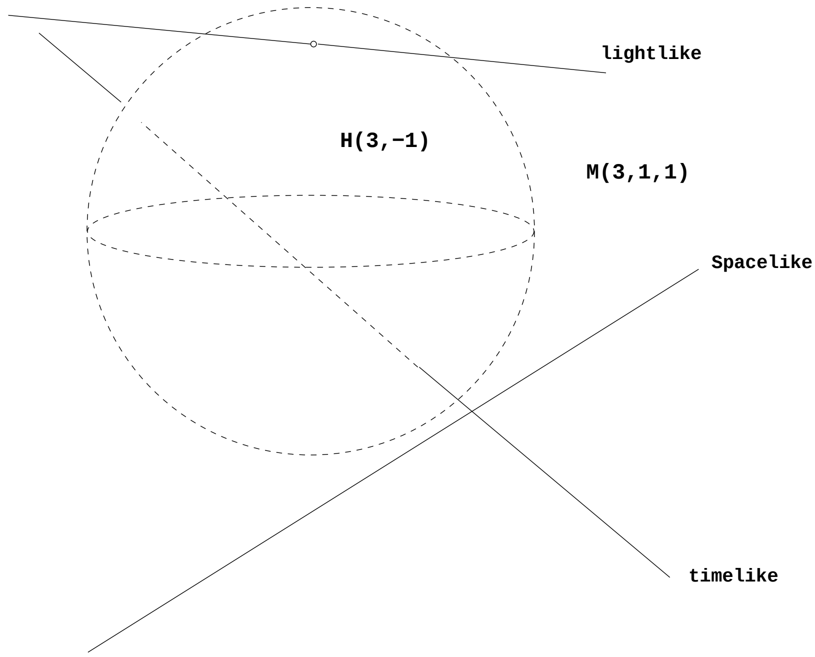
The *length* of a geodesic segment $\gamma : [a,b] \to \mathbb{M}(n,\nu,\kappa)$ is the number:

$$l(\gamma) := \int_a^b \sqrt{\langle\gamma'(t), \gamma'(t)\rangle} dt \in \mathbb{R}_+ \cup \mathbf{i}\mathbb{R}_+ \tag{2.9}$$

The following property of $d_{\mathbb{C}}$ is easily verified using the characterization of geodesics discussed previously.

Proposition 4. *If p and q are geodesically connected, then $d_{\mathbb{C}}(p,q) = l(\gamma_{p,q})$, where $\gamma_{p,q}$ is a geodesic segment joining p, q such that $|l(\gamma)|$ is minimal.*

Figure 2.1: Projective model of $\mathbb{H}(3,-1)$ and an upper hemisphere of $\mathbb{M}(3,1,1)$. Geodesics are straight lines. The two spaces are separated by a sphere, not contained in any of the spaces, which corresponds to lighlike vectors in $\mathbb{R}^4_1$. This set may be regarded as the *points at infinity.*



Subspaces and Isometries In the following we will discuss subspaces of $\mathbb{M}(n,\nu,\kappa)$. For $\kappa \neq 0$ these concepts are most easily described via the ambient semi-Euclidean space, thus the discussion implicitly also includes the case $\kappa = 0$. Refer to [21] for more details.

A *subspace* $S \subset \mathbb{M} = \mathbb{M}(n,\nu,\kappa)$ can be defined as the intersection of $\mathbb{M}$ with a linear subspace[2] $\tilde{S} \subset \mathbb{R}^{n+1}_{\nu_0}$. S is then a totally geodesic submanifold. However the intersection $\tilde{S} \cap \mathbb{M}$ can have two isometric connected components. We want to include this case as a subspace. Then in every case a subspace $S \subset \mathbb{M}$ is isometric to one or two copies of $\mathbb{M}(m,\mu,\kappa)$, for some $m < n$ and $\mu \leq \nu$.

The antipodal isometry When S is disconnected, the two connected components are interchanged by the *antipodal map*:

$$\tilde{\sigma}_A : \tilde{p} \mapsto -\tilde{p}, \tag{2.10}$$

which restricts to an isometry $\sigma_A : \mathbb{M} \to \mathbb{M}$, when the hyperquadric defining $\mathbb{M}$ is connected, that is for $\kappa < 0$, $\nu \neq 0$ and $\kappa > 0$, $\nu \neq n$ (and also for $\kappa = 0$).

[2]Recall that we use a tilde, e.g. $\tilde{S}$, to denote "objects" in $\mathbb{R}^{n+1}_{\nu_0}$ corresponding to an "object" in $\mathbb{M}(n,\nu,\kappa)$ by intersection.

A subspace S of $\mathbb{M} = \mathbb{M}(n, \nu, \kappa)$ is nondegenerate if the metric tensor restricted to TS is nondegenerate. This is the case iff the linear subspace $\tilde{S}$ such that $S = \tilde{S} \cap \mathbb{M}$ is nondegenerate iff $\tilde{S}^{\perp} \cap \tilde{S} = \emptyset$ iff $\mathbf{C}_{\kappa}(X) = \kappa \mathbf{G}_{\tilde{X}}$ is nonsingular, when $\tilde{X}$ is a basis for $\tilde{S}$.

For any subset $X \subseteq \mathbb{M}(n, \nu, \kappa)$ there is a *minimal subspace* containing X, denote this by S_X; simply define $S_X := \bigcap\{S | \ S \text{ a subspace containing } X\}$, then

$$S_X = \operatorname{span}(\tilde{X}) \cap \mathbb{M}(n, \nu, \kappa) \tag{2.11}$$

If B is subset of X, such that $\tilde{S}_X = \operatorname{span}(\tilde{X}) = \operatorname{span}(\tilde{B})$, we will also say that B spans S_X, and likewise B is a basis for S_X if $\tilde{B}$ is a basis for $\tilde{S}_X$. If S_X is nondegenerate, B is a maximal subset in X with the property that $\mathbf{G}_{\tilde{B}} = \frac{1}{\kappa}\mathbf{C}_{\kappa}(B)$ is regular.

These characterizations reduces questions on dimension of subspaces to linear algebra. See [2] for further discussions on this.

We shall denote the semi-Riemannian isometry group of $\mathbb{M} = \mathbb{M}(n, \nu, \kappa)$ by $\mathrm{Isom}(\mathbb{M})$; this consists of diffeomorphisms $\sigma : \mathbb{M} \to \mathbb{M}$ that preserves the metric tensor. For $\kappa \neq 0$, $\mathrm{Isom}(\mathbb{M})$ coincides with $O(n+1, \nu_0)$ or the subgroup of this, that preserves the connected component of the hyperquadric defining $\mathbb{M}$ (when this is not connected). See the discussion in [21], Chapter 9.

Proposition 5 (Homogeneity). *Put* $\mathbb{M} = \mathbb{M}(n, \nu, \kappa)$. *Let* $X \subseteq \mathbb{M}$ *and* $Y \subseteq \mathbb{M}$ *be subsets such that* S_X *and* S_Y *are nondegenerate. Then*

$$(X, d_{\mathbb{C}}) \underset{isom}{\cong} (Y, d_{\mathbb{C}}) \text{ iff } \sigma(X) = Y, \tag{2.12}$$

for some semi-Riemannian isometry $\sigma \in \mathrm{Isom}(\mathbb{M})$.

Proof. First assume that $\kappa \neq 0$. An element $\sigma \in \mathrm{Isom}(\mathbb{M})$ preserves the scalar product of the ambient space, hence it is clear from the definition of $d_{\mathbb{C}}$, that σ gives a $d_{\mathbb{C}}$-isometry.

Assume then that $\sigma : X \to Y$ is a $d_{\mathbb{C}}$-isometry (Definition 3). This means again by the definition of $d_{\mathbb{C}}$ that $\langle \tilde{p}, \tilde{q} \rangle = \langle \widetilde{\sigma(p)}, \widetilde{\sigma(q)} \rangle$ for any $p, q \in X$. Choose a basis for $B \subseteq X$ for S_X (i.e. a minimal subset spanning S_X). Then the Gram matrix $\mathbf{G}_{\tilde{B}}$ is regular (nondegeneracy), and $B \subseteq X$ is a maximal subset such that this is true (i.e. there are no extensions with regular Gram matrix).

But then $\widetilde{\sigma(B)}$ is a linearly independent set of vectors, since $\mathbf{G}_{\widetilde{\sigma(B)}} = \mathbf{G}_{\tilde{B}}$. And $\sigma(B)$ also spans S_Y, since if there were an extra independent point/vector $p \in Y \setminus \sigma(B)$, the preimage of this would also be independent of B in S_X (meaning that the Gram matrix of $B \cup \{\sigma^{-1}(p)\}$ would be regular). Hence $\dim(S_X) = \dim(S_Y)$.

Since σ maps a basis to a basis, there is at most one linear map $\tilde{\sigma} : \tilde{S}_X \to \tilde{S}_Y$, that extends σ. But in fact defining $\tilde{\sigma}$ to be the extension of $\sigma : B \to \sigma(B)$, does extend $\sigma : X \to Y$, since any point $r \in S_X$ is uniquely determined by the vector of scalar products with $\tilde{B}$, by nondegeneracy. Clearly $\tilde{\sigma}$ preserves the scalar product $\langle \cdot, \cdot \rangle$ of the ambient space. Then one can extend $\tilde{\sigma}$ to be an element of the required isometry group by choosing to map an ONB of $\tilde{S}_X^{\perp}$ to a suitable ONB of $\tilde{S}_Y^{\perp}$. (such that the connected component of the hyperquadric is preserved, when this is disconnected).

For $\kappa = 0$ we can choose a $p \in X$ and translations such that p and $\sigma(p)$ are at the origin. Then the argument above goes through, when we refer to Gram matrices of $X \setminus \{p\}$ and $Y \setminus \{\sigma(p)\}$. See the proof of Theorem 1 below. □

Examples show that it is necessary to require that S_X and S_Y are nondegenerate; it is possible to have isometric subsets, such that there is no global isometry with $\sigma(X) = Y$, if either S_X or S_Y is degenerate.

Recall from Definition 3 that if a distance space X is realizable as a subset of another distance space Y, we write $X \overset{isom}{\hookrightarrow} Y$. A realization $\phi : X \overset{isom}{\hookrightarrow} \mathbb{M}(n, \nu, \kappa)$ is called *minimal* if X is not realizable in any $\mathbb{M}(m, \mu, \kappa)$ with $m < n$. It follows from Theorem 1 below, that for a minimal realization ν is determined by m and κ. In the light of Proposition 5, we may then speak of *the* minimal realization:

Proposition 6. *Let X be a finite $\mathbb{C}_\kappa$-distance space with distance matrix $\mathbf{D} \in \mathcal{D}_n(\mathbb{C}_\kappa)$. A minimal realization $\phi : X \overset{isom}{\hookrightarrow} \mathbb{M}(n, \nu, \kappa)$ is unique up to isometry of $\mathbb{M}(n, \nu, \kappa)$.*

Proof. We only have to show, that for a minimal realization the subspace $S_{\phi(X)}$ is nondegenerate, then the result follows from Proposition 5. That $S_{\phi(X)}$ is nondegenerate will follow from Theorem 1 below. □

There are various equivalent formulations of the criterion for when a finite distance space X is realizable as a subset of $\mathbb{M}(n, \nu, \kappa)$. They go back to the work of Schoenberg, Menger and Blumenthal in the 1930's, see [2],[28], but seem to be rediscovered from time to time in different contexts. Here we shall work with the $\mathbf{C}_\kappa(X)$-matrix.

The following result is an easy extension of the ideas found in [28].

Theorem 1. *Let $X = \{p_1, \ldots, p_n\}$ be a finite distance space with distance matrix $\mathbf{D}$. $X \overset{isom}{\hookrightarrow} \mathbb{M}(m, \nu, \kappa)$ if and only if*

$$\mathbf{D} \in \begin{cases} \mathcal{D}_n(\mathbb{R}_+) & \text{if } \nu = 0 \\ \mathcal{D}_n(\mathbf{i}\mathbb{R}_+) & \text{if } \nu = m \\ \mathcal{D}_n(\mathbb{C}_\kappa) & \text{otherwise}, \end{cases} \tag{2.13}$$

and we have

- $n_- \leq \nu$ *and* $n_+ \leq m + 1 - \nu$, *if* $\kappa > 0$.
- $n_- \leq \nu + 1$ *and* $n_+ \leq m - \nu + 1$, *if* $\kappa = 0$.
- $n_- \leq m - \nu$ *and* $n_+ \leq \nu + 1$, *if* $\kappa < 0$.

where (n_-, n_+, n_0) *is the signature of* $\mathbf{C}_\kappa(X)$ *if* $\kappa \neq 0$ *and the signature of* $\mathbf{I}_1\mathbf{C}_0(X)$ *if* $\kappa = 0$.

Furthermore in case $X \overset{isom}{\hookrightarrow} \mathbb{M}(n, \nu, \kappa)$, *then the minimal m such that* $X \overset{isom}{\hookrightarrow} \mathbb{M}(m, \mu, \kappa)$, *for some* μ, *is, for* $\kappa \neq 0$, *equal to* $\mathrm{rank}(\mathbf{C}_\kappa(X)) - 1$, *and for* $\kappa = 0$ *equal to* $\mathrm{rank}(\mathbf{C}_0(X)) - 2$. *Such a minimal realization spans the target space:* $S_X = \mathbb{M}(m, \mu, \kappa)$.

Proof. First we will treat the case $\kappa \neq 0$.

Assume that X is a finite subset of $\mathbb{M}(m, \nu, \kappa)$, then by the definition of $d_{\mathbb{C}}$ we obtain a distance matrix with values such that (2.13) is true. And by Sylvester's Law of Inertia, Proposition 1, the claim about the signature follows immediately from (2.7).

Now for the opposite direction, assume that X is a $\mathbb{C}_\kappa$-space that satisfies the signature condition and the condition on the values of the distance, (2.13).

As on page 10, we obtain vectors $Y = \{q_1, \ldots, q_n\} \subset \mathbb{R}^{m_0}_{n_-}$, such that $\mathbf{C}_\kappa(X) \in \mathrm{Sym}_n(\mathbb{R})$ is the Gram-matrix of Y, $\mathbf{C}_\kappa(X) = \mathbf{G}_Y = [\langle q_i, q_j \rangle]$, where $m_0 = n_+ + n_- = \mathrm{rank}(\mathbf{C}_\kappa(X))$. Here $Y \subset \mathbb{M}(m_0 - 1, n_-, 1)$, since the diagonal entries of $\mathbf{C}_\kappa(X)$ are equal to 1; the assumption on the distances, (2.13), in the definite cases assures, that the points obtained are in the same connected component, when the hyperquadric is disconnected. Multiplying the scalar product by $\frac{1}{\kappa}$, Y can be interpreted as a point set of $\mathbb{M}(m_0 - 1, n_-, \kappa)$ if $\kappa > 0$ and of $\mathbb{M}(m_0 - 1, n_+ - 1, \kappa)$ if $\kappa < 0$. Since both X and Y are $\mathbb{C}_\kappa$-spaces, the periodicity is such that $d_{\mathbb{C}}(q_i, q_j) = d(p_i, p_j)$.

This is the minimal realization, $m = \mathrm{rank}(\mathbf{C}_\kappa(X)) - 1$, since otherwise the Gram matrix $\mathbf{G}_Y$ would have rank less than $\mathrm{rank}(\mathbf{C}_\kappa(X))$. Clearly Y spans $\mathbb{R}^{m_0}_{\nu_0}$ since $\mathrm{rank}(\mathbf{G}_Y) = m_0$, hence $X = Y$ spans the target (and the realization is nondegenerate).

Finally: $\mathbb{M}(m_0 - 1, \nu_0, \kappa) \overset{isom}{\hookrightarrow} \mathbb{M}(m, \nu, \kappa)$ for any m, ν s.t. $m > m_0 - 1$, $\nu \geq \nu_0$ and $m - \nu \geq m_0 - 1 - \nu_0$. This settles the condition on the signature.

Then for the case $\kappa = 0$. $\mathbf{I}_1\mathbf{C}_0(X)$ means that the zeroth row of $\mathbf{C}_0(X)$ is multiplied by -1 to obtain a symmetric matrix. By elementary row and column operations, we then find that the symmetric matrix thus obtained from $\mathbf{C}_0(X)$ is equivalent to a matrix in block diagonal form:

$$\begin{pmatrix} 0 & 1 & 0 & \cdots \\ 1 & 0 & 0 & \cdots \\ 0 & 0 & \mathbf{E} & \\ \vdots & \vdots & & \end{pmatrix}, \tag{2.14}$$

where $\mathbf{E} = [e_{ij}] \in \mathrm{Sym}_{n-1}(\mathbb{R})$ is the matrix obtained by forming "cosine-relations" with p_1 as base point: $e_{ij} = \frac{1}{2}(d^2_{1,i+1} + d^2_{1,j+1} - d^2_{i+1,j+1})$.

Consider $\mathbf{E}$ as a Gram-matrix of a subset of some $\mathbb{R}^m_\nu$, $\tilde{X} = \{\tilde{p}_2, \ldots, \tilde{p}_n\} \subset \mathbb{R}^m_\nu$: $e_{ij} = \langle \tilde{p}_{i+1}, \tilde{p}_{j+1} \rangle$, and compare with the definition of the distance, Definition 11. It is then easy to see that this gives a realization with $\phi(p_1) = 0$ and $\phi(p_i) = \tilde{p}_i$ for $i > 1$.

But this is possible iff $m \geq \mathrm{rank}(\mathbf{E}) = \mathrm{rank}(\mathbf{C}_0(X)) - 2$, $\nu \geq \iota(\mathbf{E}) = n_- - 1$ and $m - \nu \geq \rho(\mathbf{E}) = n_+ - 1$. Again we see that the minimal realization is in dimension

$\mathrm{rank}(\mathbf{E}) = \mathrm{rank}(\mathbf{C}_0(X)) - 2$, exactly when the realization of X spans the target. Compare with [28]. □

Remark 6. Note that $\det(\mathbf{I}_1\mathbf{C}_0(X)) = -\det(\mathbf{C}_0(X))$ and then from Theorem 1 it follows that for all κ and a subset $X \subset \mathbb{M}(m, \nu, \kappa)$ having $\det(\mathbf{C}_\kappa(X)) \neq 0$ requires $m \geq |X| - 1$. (This also follows directly from the interpretation of $\mathbf{C}_\kappa(X)$ as a Gram-matrix, Remark 5.) This will be the most important ingredient in the proof of Theorem 2.

2.3 Geometry of Simplices in $\mathbb{M}(n, \nu, \kappa)$

In this section we shall treat the geometry of (generalized) simplices in $\mathbb{M}(n, \nu, \kappa)$, and establish a formula which shows the geometric significance of $\det(\mathbf{C}_\kappa(X))$. This is just an extension of a well known formula for the Cayley-Menger matrix, see [2].

Reflections and Altitudes The reflection in (or symmetry of) a nondegenerate subspace S is the unique isometry $\sigma_S \in \mathrm{Isom}(\mathbb{M})$ such that $S = \mathrm{fix}(\sigma_S) := \{p \in \mathbb{M} | \, \sigma_S(p) = p\}$ and $\sigma_{S*} = -id$ on TS. It is induced by a reflection in $\tilde{S}$ in the ambient semi-Euclidean space, which can be described as the map $\tilde{\sigma}_{\tilde{S}} \in O(n+1, \nu_0)$ such that

$$v \mapsto \pi(v) - \pi^{\perp}(v), \tag{2.15}$$

where $\pi : \mathbb{R}^{n+1}_{\nu_0} \to \tilde{S}$ is the orthogonal projection onto $\tilde{S}$ and $\pi^{\perp} : \mathbb{R}^{n+1}_{\nu_0} \to \tilde{S}^{\perp}$ is the projection onto the orthogonal complement (cf. [21] p.50) . Then $\sigma_S = \tilde{\sigma}_{\tilde{S}}$ restricted to $\mathbb{M}$.

Lemma 5. *Let V be nondegenerate linear subspace of $\mathbb{R}^{n+1}_{\nu}$ and let $\tilde{\sigma}_V$ be the reflection in V,* (2.15)*. Then for any $v \in \mathbb{R}^{n+1}_{\nu} \setminus V$ such that $W = \mathrm{span}(V \cup \{v\})$ is nondegenerate the geodesic connecting v and $\tilde{\sigma}_V(v)$ is not lightlike.*

Proof. We have $\pi^{\perp}(v) = v - \pi(v) \in V^{\perp} \cap W$, but since $V \subset W$ is a nondegenerate subspace of W, which is also a nondegenerate space, then $V^{\perp} \cap W$ is one dimensional and nondegenerate. But then $\langle v - (\pi(v) - \pi^{\perp}(v)), v - (\pi(v) - \pi^{\perp}(v)) \rangle = 4\langle \pi^{\perp}(v), \pi^{\perp}(v) \rangle \neq 0$. □

We define the altitude from $p \in \mathbb{M}$ onto S as

$$d_{\mathbb{C}}(p, S) := \frac{1}{2} d_{\mathbb{C}}(p, \sigma_S(p)) \in \frac{1}{2}\mathbb{C}_\kappa \tag{2.16}$$

Example 1. For $\mathbb{M} = \mathbb{S}(n, 1)$ and $S = \{p, q\}$, where p and q are antipodal, σ_S is the rotation in $SO(n+1)$ which fixes p, q and corresponds to the antipodal map σ_A on the equatorial $\mathbb{S}(n-1, 1)$. Hence the altitude $d_{\mathbb{C}}(p, S)$ is equal to the "latitude" of p, the distance to the closest "pole", which is then $\frac{\pi}{2}$ on the equator and in $[0, \frac{\pi}{2})$ on the two open hemispheres. Note that for p not on the equator, there is a well defined map taking p to the closest point in S, this is the *orthogonal projection*.

In case p and $\sigma_S(p)$ are not geodesically connected or are antipodal, there is no immediate way to define the orthogonal projection of p onto S. But otherwise, we have an orthogonal projection, which can be described as:

Put $l = 2|d_{\mathbb{C}}(p, S)|$, and let $\gamma : [0, l] \to \mathbb{M}$ be the unique geodesic with $\gamma(0) = p$ and $\gamma(l) = \sigma_S(p)$. Then $p_S = \gamma(\frac{l}{2}) \in S$, and γ intersects S orthogonally. We then have $d_{\mathbb{C}}(p, S) \in \mathbb{R}_+^*$ iff γ is spacelike and nontrivial, $d_{\mathbb{C}}(p, S) \in \mathbf{i}\mathbb{R}_+^*$ iff γ is timelike and $d_{\mathbb{C}}(p, S) = 0$ iff $p \in S$ or γ is lightlike. This follows easily from Proposition 3.

Definition 12 (Generalized Simplices). Let $X = \{p_1, \dots, p_{n+1}\} \subset \mathbb{M}(m, \nu, \kappa)$.

- X is said to be the vertex set of a simplex if $\det(\mathbf{C}_\kappa(X)) \neq 0$.
- X is said to have nondegenerate faces if for every $Y \subseteq X$ we have $\det(\mathbf{C}_\kappa(Y)) \neq 0$.

We also say that X span a simplex, and that a subset $Y \subset X$ span a face of codimension $|X \setminus Y|$.

From now on we shall loosen the terminology and not distinguish between a simplex and its set of vertices X; likewise for faces, which are simplices in their own right.

Using Theorem 1 it can be seen that all simplices in the Riemannian cases, $\nu = 0$, must have nondegenerate faces. In these cases we will use $\Delta(X)$ to denote the convex hull of $X \subseteq \mathbb{M}(n, \kappa)$, which in this context usually means the "simplex spanned by X".

From the previous discussion of subspaces we see that the requirement that a simplex X has nondegenerate faces corresponds to saying that for any $Y \subseteq X$,

$$S_Y \text{ is nondegenerate and } Y \text{ is a basis for } S_Y$$

Assume that $X = \{p_1, \dots, p_{n+1}\} \subset \mathbb{M}(n, \nu, \kappa)$ span a simplex with *nondegenerate faces*. Every points $p_i \in X$ has an altitude h_i, onto the subspace S_{X_i}, spanned by the points $X_i := X \setminus \{p_i\}$. For $i \in \{2, \dots, n+1\}$, we will use $h_{<i}$ to denote the altitude of p_i in the subsimplex spanned by $\{p_1, \dots, p_{i-1}\}$. Hence

$$h_{<2} = d_{\mathbb{C}}(p_2, p_1) \text{ or } h_{<2} = d_{\mathbb{C}}(p_2, \sigma_A(p_1)) = \frac{\pi}{\sqrt{\kappa}} - d_{\mathbb{C}}(p_2, p_1),$$

where σ_A is the antipodal isometry (in the cases, where this exists).

Lemma 6. *Let $X = \subset \mathbb{M}(n, \nu, \kappa)$ span a simplex with nondegenerate faces. Then for every $Y \subset X$ and $p \in X \setminus Y$ the altitude from p onto the subspace spanned by Y is nonvanishing: $d_{\mathbb{C}}(p, S_Y) \neq 0$.*

Proof. Since $p \notin S_Y$, the only way we can get $d_{\mathbb{C}}(p, S_Y) = 0$ is if p and $\sigma_{S_Y}(p)$ are connected by a lightlike geodesic. However every lightlike geodesic γ corresponds to a lightlike geodesic $\tilde{\gamma}$ of the ambient space (see [21] 4.28), and this would then have to connect $\tilde{\sigma}_{\tilde{S}_Y}(\tilde{p})$ and $\tilde{p}$. This is impossible by Lemma 5 since $\tilde{S}_Y$ is nondegenerate and likewise for $\tilde{S}_{Y \cup \{p\}} = \mathrm{span}(\tilde{Y} \cup \{\tilde{p}\})$, corresponding to the face $Z = Y \cup \{p\} \subseteq X$. $\square$

We have the following interesting trigonometric formula:

Theorem 2. *Let $X = \{p_1, \dots, p_{n+1}\} \subset \mathbb{M}(n, \nu, \kappa)$ span a simplex with nondegenerate faces. Then:*

$$\det(\mathbf{C}_\kappa(X)) = \prod_{i=2}^{n+1} \mathbf{s}_\kappa(h_{<i})^2 \tag{2.17}$$

Proof. Let p_{n+2} be the reflection of p_{n+1} in the hypersurface M_{n+1} containing $X_{n+1} := X \setminus \{p_{n+1}\}$.
Then $d(p_{n+1}, p_{n+2}) = 2h_{n+1}$, and $d(p_i, p_{n+2}) = d(p_i, p_{n+1})$ for $i \neq n+1$, where h_{n+1} denotes the altitude from p_{n+1} onto M_{n+1}. Let $\hat{X}$ be $X \cup \{p_{n+2}\}$. Since $|\hat{X}| = n+2$, and $\hat{X} \subset \mathbb{M}(n, \nu, \kappa)$, the $\mathbf{C}_\kappa(\hat{X})$-matrix must be singular. Now the two last columns and the two last rows of $\mathbf{C}_\kappa(\hat{X})$ are identical, except for inside the principal 2×2-submatrix which involves p_{n+1} and p_{n+2}:

$$\begin{pmatrix} 1 & \mathbf{c}_\kappa(2h_{n+1}) \\ \mathbf{c}_\kappa(2h_{n+1}) & 1 \end{pmatrix} \tag{2.18}$$

We see that $|\mathbf{C}_\kappa(\hat{X})_{n+1}| = |\mathbf{C}_\kappa(\hat{X})_{n+2}| = |\mathbf{C}_\kappa(X_{n+1})|$ and $|\mathbf{C}_\kappa(\hat{X})^{n+2}_{n+1}| = |\mathbf{C}_\kappa(X)| + (\mathbf{c}_\kappa(2h_{n+1}) - 1)|\mathbf{C}_\kappa(X_{n+1})|$ (simply expand the minor). Hence applying formula (1.8), we get (since $|\mathbf{C}_\kappa(\hat{X})| = 0$):

$$|\mathbf{C}_\kappa(X)|^2 = (|\mathbf{C}_\kappa(X)| + (\mathbf{c}_\kappa(2h_{n+1}) - 1)|\mathbf{C}_\kappa(X_{n+1})|)^2$$

We have $(\mathbf{c}_\kappa(2h_{n+1}) - 1)|\mathbf{C}_\kappa(X_{n+1})| \neq 0$ since X_{n+1} span a simplex and $\mathbf{c}_\kappa(2h_{n+1}) \neq 1$ by the previous lemma. Using this we obtain from the equation above:

$$\frac{1}{2}(1 - \mathbf{c}_\kappa(2h_{n+1}))|\mathbf{C}_\kappa(X_{n+1})| = |\mathbf{C}_\kappa(X)|$$

We have the usual formula:

$$1 - \mathbf{c}_\kappa(2h_{n+1}) = 2\mathbf{s}_\kappa(h_{n+1})^2, \tag{2.19}$$

valid for complex numbers as well (by analytic continuation). Inserting this we obtain:

$$\mathbf{s}_\kappa(h_{n+1})^2|\mathbf{C}_\kappa(X_{n+1})| = |\mathbf{C}_\kappa(X)| \tag{2.20}$$

Note that for $\kappa = 0$ everything goes through with the convention $\mathbf{c}_0(x) := 1 - \frac{x^2}{2}$, $\mathbf{s}_0(x) := x$. The result follows by induction, since $|\mathbf{C}_\kappa(\{p_1\})| = 1$. □

Remark 7. It is interesting to note that since the left hand side of the formula is independent of the ordering of the points, this is also true for the right hand side. Also the proof actually doesn't require that all faces are nondegenerate, but only that we have an increasing sequence: $X^2 = \{p_1, p_2\} \subset X^3 \subset \cdots \subset X^{n+1} = X$ of nondegenerate faces with $|X^{i+1}| = |X^i| + 1$. (We can loosen this and not require $X = X^{n+1}$ nondegenerate:

then the last altitude is zero, as is easily seen from Lemma 5, and the equation just reads $0 = 0$.)

Also note that, for $\kappa \neq 0$, everything is "antipodally invariant": Mapping a point p_i to its antipode $\sigma_A(p_i)$ will alter the altitude from p_i as: $h_i \mapsto \frac{\pi}{\sqrt{\kappa}} - h_i$, but this does not change $\mathbf{s}_\kappa(h_i)$, hence doesn't change the determinant; this is also seen directly since mapping p_i to its antipode corresponds to changing a sign in row and column i of $\mathbf{C}_\kappa(X)$.

With this theorem, we have a another formulation of Heron's Formula (1.10):

Proposition 7 (Heron's Formula). *Let $X = \{p_1, p_2, p_3\} \subset \mathbb{M}(n, \nu, \kappa)$ be a triangle with edge lengths:*

$$d_{\mathbb{C}}(p_1, p_2) = a,\ d_{\mathbb{C}}(p_2, p_3) = b,\ d_{\mathbb{C}}(p_3, p_1) = c,$$

and put $s = \frac{1}{2}(a + b + c)$. Then if $a \neq 0$:

$$\mathbf{s}_\kappa(a)^2 \mathbf{s}_\kappa(h)^2 = 4\,\mathbf{s}_\kappa(s)\mathbf{s}_\kappa(s-a)\mathbf{s}_\kappa(s-b)\mathbf{s}_\kappa(s-c), \tag{2.21}$$

where h is the altitude from p_3.

Proof. This follows directly from Theorem 2 and Heron's Formula (and the remark above on antipodality). □

The following example is quite illustrative and will appear in various forms throughout this thesis.

Example 2 (Regular Simplices). A regular simplex $X \subset \mathbb{M}(n, \nu, \kappa)$ is a simplex where all edge lengths d_{ij} are equal to the same constant l. The $\mathbf{C}_\kappa(X)$ matrix of such a simplex has the form:

$$\begin{pmatrix} 1 & \mathbf{c}_\kappa(l) & \mathbf{c}_\kappa(l) & \dots \\ \mathbf{c}_\kappa(l) & 1 & \mathbf{c}_\kappa(l) & \dots \\ \mathbf{c}_\kappa(l) & \mathbf{c}_\kappa(l) & 1 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{2.22}$$

Expanding this $(n+1) \times (n+1)$ determinant, we obtain:

$$\det(\mathbf{C}_\kappa(X)) = (1 - \mathbf{c}_\kappa(l))^n (n\mathbf{c}_\kappa(l) + 1) \tag{2.23}$$

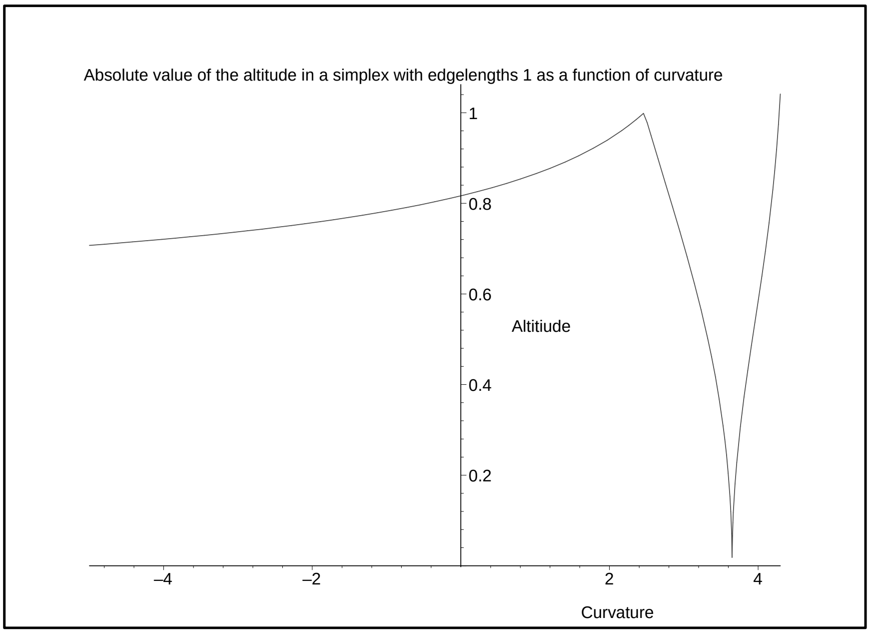
It can also be checked that this factorization of the determinant corresponds to the eigenvalues of $\mathbf{C}_\kappa(X)$. We see that the matrix is singular exactly when $\mathbf{c}_\kappa(l) = -\frac{1}{n}$. This corresponds to the fact, that we can embed a metric space with all distances equal to l as a regular simplex in $\mathbb{S}(1, \kappa)$ iff $l < \mathbf{c}_\kappa^{-1}(\frac{-1}{n})$, and if $l = \mathbf{c}_\kappa^{-1}(-\frac{1}{n})$ we can embed the space with a *dimension drop* of 1 in $\mathbb{S}(n-1, \kappa)$. When $-1 \leq \mathbf{c}_\kappa(l) < -\frac{1}{n}$, $\mathbf{C}_\kappa(X)$ has exactly one negative eigenvalue, and X is realizable in $\mathbb{M}(n, 1, \kappa)$.

Using (2.20), we obtain a formula for the altitude from a vertex of X onto the opposite face:

$$\mathbf{s}_\kappa(h)^2 = (1 - \mathbf{c}_\kappa(l)) \frac{n\mathbf{c}_\kappa(l) + 1}{(n-1)\mathbf{c}_\kappa(l) + 1} \tag{2.24}$$

Note that $\mathbf{s}_\kappa(h)^2$ is negative when h is real and $\kappa < 0$ by the definition of $\mathbf{s}_\kappa$, (1.6). See a plot of the altitude as a function of curvature in Figure 2.3.

Figure 2.2: A plot of the absolute value of the altitude in a regular 3-dimensional simplex with edge lengths 1. Note that the simplex collapses for $\kappa = \mathrm{Arccos}(-\frac{1}{3})^2$, after this the altitude becomes imaginary.



2.4 Duality

For all $\mathbb{M}(n, \kappa)$ there is a duality, which for points $p, q \in \mathbb{M}(n, \kappa)$ gives subsets $\overset{**}{p}, \overset{**}{q}$ in a dual space $\mathbb{M}^*$ such that $d(p, q) = \mu(\overset{**}{p} \triangle \overset{**}{q})$, where μ is a measure on $\mathbb{M}^*$. This fact will be important later in the discussion of *negative type*, chapter 4. It is a duality which appears in different disguises in e.g. [26],[27],[24],[29],[30] and [31]. We refer to these for more details and alternative descriptions.

The duality can be viewed as an instance the "orthogonal complement duality" in the ambient $\mathbb{R}^{n+1}_\nu$, which maps a set V to

$$V^\perp = \{w \in \mathbb{R}^{n+1}_\nu \mid \langle w, v \rangle = 0, \forall v \in V\} \tag{2.25}$$

However it can also be studied from a purely intrinsic point of view. And the intrinsic formulation has a translation in a quite different setting, namely for *weighted trees*, another important class of metric spaces.

It is possible to formulate the duality in full generality for all $\mathbb{M}(n, \nu, \kappa)$, but it is then most easily studied via the HS-spaces defined by Schlenker in [29], where the two hyperquadrics in $\mathbb{R}^{n+1}_\nu$ are joined into a single space. Here we shall primarily be interested in the Riemannian space forms $\mathbb{M}(n, \kappa)$.

Dihedral Angles & Gram Matrix Duality

We shall give version of the duality referred to above, as a duality between simplices that interchange edge lengths and dihedral angles. This can be stated in a very explicit way in terms of the $\mathbf{C}_\kappa$-matrix of a simplex.

Assume that $X = \{p_1, \ldots, p_{n+1}\} \subset \mathbb{M}(n, \kappa)$ span a simplex. The boundary of the convex hull $\partial\Delta(X)$, which is the union of codimension 1 faces, is homeomorphic to $\mathbb{S}^{n-1}$ and divides $\mathbb{M}(n, \kappa)$ into two components, one of which (the "inside") has strictly less volume than the other (the "outside").

For i and j in $\{1, \ldots, n+1\}$, the codimension 1 faces $\Delta(X_i)$ and $\Delta(X_j)$ intersect along the codimension 2 face $\Delta(X_{ij})$, at an exterior *dihedral angle* θ_{ij} which is defined to be $\operatorname{ang}(n_i, n_j)$. Here $\operatorname{ang}(n_i, n_j)$ is the distance between the *outward* pointing normal vectors in the unit sphere of $T_p\mathbb{M}(n, \kappa)$, where $p \in \Delta(X_{ij})$. Note that with this definition $\theta_{ii} = 0$.

Dihedral Gram Matrix The matrix $[\cos(\theta_{ij}]$ of cosines to the exterior dihedral angles is sometimes called the Gram matrix of the simplex, c.f. [20], since it is equal to the Gram matrix of the set of outward pointing normals. We shall call this matrix, the *dihedral Gram matrix*.

Proposition 8. *Let $X = \{p_1, \ldots, p_{n+1}\}$ be points of $\mathbb{M}(n, \kappa)$ such that $\mathbf{C}_\kappa(X)$ is regular, i.e. the points span a simplex. Let $[c_{ij}]$ be the elements of the cofactor matrix*[3] $\operatorname{cof}(\mathbf{C}_\kappa(X))$ *of $\mathbf{C}_\kappa(X)$. The exterior dihedral angles θ_{ij} satisfy:*

$$\cos(\theta_{ij}) = \frac{c_{ij}}{\sqrt{c_{ii}}\sqrt{c_{jj}}}, \tag{2.26}$$

where the convention $\sqrt{z} \in \mathbb{R}_+ \cup \mathbf{i}\mathbb{R}_+$ for $z \in \mathbb{R}^*$ is used.

Proof. Consider the points $p_i, p_j \in X$, $i \neq j$. Let h_i be the altitude from p_1 onto the subspace M_i spanned by $X_i = X \setminus \{p_i\}$, and let h_{ij} be the altitude onto the subspace M_{ij} spanned by $X_{ij} = X_i \setminus \{p_j\}$. Then $h_{ij} > h_i$ and we have a right angled triangle with vertices p_i, f_i, f_{ij}, where f_i is the point closest to p in M_i and f_{ij} the closest point in M_{ij}. Now the angle of this triangle at the vertex f_{ij} is seen to be either the interior or the exterior dihedral angle θ_{ij}. By the sine relation (2.3), we have $\sin(\pi - \theta_{ij}) = \sin(\theta_{ij}) = \frac{\mathbf{s}_\kappa(h_i)}{\mathbf{s}_\kappa(h_{ij})}$.

Using (1.8) we get: $\frac{|\mathbf{C}_\kappa(X)^i_j|^2}{|\mathbf{C}_\kappa(X_i)||\mathbf{C}_\kappa(X_j)|} = 1 - \frac{|\mathbf{C}_\kappa(X)||\mathbf{C}_\kappa(X_{ij})|}{|\mathbf{C}_\kappa(X_i)||\mathbf{C}_\kappa(X_j)|}$. X_{ij} is a subset of X_j, so using (2.20) we get $|\mathbf{C}_\kappa(X_j)| = \mathbf{s}_\kappa(h_{ij})^2|\mathbf{C}_\kappa(X_{ij})|$. Similarly $|\mathbf{C}_\kappa(X)| = \mathbf{s}_\kappa(h_i)^2|\mathbf{C}_\kappa(X_i)|$. Inserting we get:

$$\frac{c_{ij}^2}{c_{ii}c_{jj}} = \frac{|\mathbf{C}_\kappa(X)^i_j|^2}{|\mathbf{C}_\kappa(X_i)||\mathbf{C}_\kappa(X_j)|} = 1 - \frac{\mathbf{s}_\kappa(h_i)^2}{\mathbf{s}_\kappa(h_{ij})^2} = 1 - \sin(\theta_{ij})^2 = \cos(\theta_{ij})^2 \tag{2.27}$$

[3] see the preliminaries chapter

Hence the formula is established up to a sign. In every case an easy analysis of a regular simplex, where all distances and dihedral angles are equal, shows that here the sign in (2.26) is right. During a smooth deformation of the simplex (i.e. the edge lengths and dihedral angles varying smoothly) (2.26) will vary smoothly. This shows, that the sign in (2.26) remains valid for all simplices. □

Looking at the formula in Proposition 8 it is tempting to use it as a definition of dihedral angles in the semi-Riemannian space forms $\mathbb{M}(n,\nu,\kappa)$, thus obtaining dihedral angles with complex values, as for the distance $d_{\mathbb{C}}$. We shall not pursue this further here. However we will briefly study the "duality" map:

$$\Psi : \mathbf{X} \mapsto \Lambda^{-1}\operatorname{cof}(\mathbf{X})\Lambda^{-1},\ \Lambda = \operatorname{diag}(\sqrt{|\mathbf{X}_1|},\ldots,\sqrt{|\mathbf{X}_{n+1}|}), \tag{2.28}$$

defined on a suitable subset of $\mathcal{N}_n$, the affine subspace of $\mathrm{Sym}_{n+1}(\mathbb{R})$ consisting of unidiagonal matrices:

$$\mathcal{N}_n := \{[x_{ij}] \in \mathrm{Sym}_{n+1}(\mathbb{R}) \mid x_{ii} = 1\,\forall i\}$$

Here we will consider the following subsets, which have the most important interpretations for our purposes, c.f. [20]:

$$\begin{aligned} C_n^+ &:= \{\mathbf{X} \in \mathcal{N}_n \cap \mathrm{Gl}_{n+1}(\mathbb{R}) \mid \iota(\mathbf{X}) = 0 \text{ i.e. } \mathbf{X} \text{ positive definite }\} \\ C_n^- &:= \{\mathbf{X} \in \mathcal{N}_n \cap \mathrm{Gl}_{n+1}(\mathbb{R}) \mid \iota(\mathbf{X}) = 1 \text{ and } \operatorname{cof}(\mathbf{X}) \text{ has only positive entries}\} \\ H_n &:= \{\mathbf{X} \in \mathcal{N}_n \cap \mathrm{Gl}_{n+1}(\mathbb{R}) \mid \iota(\mathbf{X}) = n \text{ and } \mathbf{X} \text{ has only positive entries }\} \end{aligned}$$

We will show:

Proposition 9. $\Psi : C_n^+ \cup C_n^- \cup H_n \to C_n^+ \cup C_n^- \cup H_n$ *is a diffeomorphism satisfying* $\Psi \circ \Psi = id$ *and*

$$\Psi(C_n^+) = C_n^+ \quad \Psi(H_n) = \Psi(C_n^-) \text{ and } \Psi(C_n^-) = H_n$$

Furthermore:

- *For every* $\mathbf{X} \in C_n^+$ *there is a unique simplex in* $X \subset \mathbb{S}(n,1)$ *such that* $\mathbf{C}_\kappa(X) = \mathbf{X}$ *and a unique simplex* $X^* \subset \mathbb{S}(n,1)$ *such that* $\mathbf{X}$ *is the dihedral Gram matrix of* X^*.
- *For every* $\mathbf{X} \in H_n$ *there is a unique simplex* $X \subset \mathbb{H}(n,-1)$ *such that* $\mathbf{X} = \mathbf{C}_\kappa(X)$.
- *For every* $\mathbf{X} \in C_n^-$ *there is a unique simplex* $X \subset \mathbb{M}(n,1,1)$ *such that* $\mathbf{X} = \mathbf{C}_\kappa(X)$ *and a unique simplex* $X^* \subset \mathbb{H}(n,-1)$ *such that* $\mathbf{X}$ *is the dihedral Gram matrix of* X^*.

Proof. For an invertible matrix $\mathbf{X} \in \mathrm{Gl}_{n+1}(\mathbb{R})$ we have: $\operatorname{cof}(\mathbf{X}) = |\mathbf{X}|\mathbf{X}^{-1}$. Hence the map Ψ can also be described as

$$\Psi(\mathbf{X}) = \mathbf{N}\mathbf{X}^{-\mathbf{1}}\mathbf{N}, \tag{2.29}$$

where $\mathbf{N}$ is a unique, diagonal normalization matrix, determined by the requirement that the diagonal elements of $\Psi(\mathbf{X})$ are 1. Hence

$$\mathbf{N} = \mathrm{diag}(\sqrt{\frac{|\mathbf{X}|}{|\mathbf{X}_i|}}, \ldots, \sqrt{\frac{|\mathbf{X}|}{|\mathbf{X}_{n+1}|}}), \tag{2.30}$$

which makes sense when all the principal minors $|\mathbf{X}_i|$ are nonvanishing and have the same sign. This is the case for C_n^- by definition and for C_n^+ by properties of positive definite matrices. For H_n it follows[4] that all principal minors of same size are nonvanishing and of same sign, when it is established that these matrices are $\mathbf{C}_\kappa$-matrices of hyperbolic simplices; this is done below. Hence Ψ is defined on $C_n^+ \cup C_n^- \cup H_n$.

Whenever Ψ is well defined for $\mathbf{X}$, we have $\Psi(\Psi(\mathbf{X})) = \Psi(\mathbf{N}\mathbf{X}^{-1}\mathbf{N}) = \hat{\mathbf{N}}\mathbf{N}^{-1}\mathbf{X}\mathbf{N}^{-1}\hat{\mathbf{N}}$, where $\hat{\mathbf{N}}$ is the uniquely determined normalization matrix, which we see must be: $\hat{\mathbf{N}} = \mathbf{N}$, so that $\Psi(\Psi(\mathbf{X})) = \mathbf{X}$. Since Ψ is clearly smooth (and its own inverse), Ψ is a diffeomorphism.

It is clear by Sylvester's Law of Inertia, that Ψ maps a positive definite matrix to a positive definite matrix, hence since Ψ is an involution $\Psi(C_n^+) = C_n^+$.

By definition all cofactors are positive for $\mathbf{X} \in C_n^-$, so since the determinant of $\mathbf{X}$ is negative, all entries of $\mathbf{X}^{-1}$ are negative. Hence the normalization (2.29), multiplies $\mathbf{X}^{-1}$ by -1 and reverses the signature (which is the same as the signature of $\mathbf{X}$), so that Ψ maps into H_n.

We have in general $\mathrm{cof}(\mathbf{N}\mathbf{X}^{-1}\mathbf{N}) = |\mathbf{N}|^2|\mathbf{X}|^{-1}\mathbf{N}^{-1}\mathbf{X}\mathbf{N}^{-1}$. In the case of $\mathbf{X} \in H_n$ all the $|\mathbf{X}_i|$ have opposite sign of $|\mathbf{X}|$, as will follow from the characterization $\mathbf{X} = \mathbf{C}_\kappa(X)$ for a hyperbolic simplex X. Using this we see that both for $|\mathbf{X}| > 0$, n even, and $|\mathbf{X}| < 0$, n uneven, we have positive cofactors of $\Psi(\mathbf{X})$ and $\Psi(\mathbf{X})$ has the opposite signature of $\mathbf{X}$. Hence $\Psi(\mathbf{X}) \in C_n^-$.

Again since Ψ is an involution we then have $\Psi(H_n) = C_n^-$ and $\Psi(C_n^-) = H_n$.

Now for the identification of the sets as $\mathbf{C}_\kappa$-matrices of simplices:

For $\mathbf{X} = [x_{ij}] \in C_n^+$, then since every 2×2-principal minor is positive definite with 1's on the diagonal, all off diagonal elements must satisfy $|x_{ij}| < 1$, hence we have d_{ij}'s such that $x_{ij} = \cos(d_{ij})$. This determines a distance space X such that $\mathbf{X} = \mathbf{C}_\kappa(X)$, and X is realizable as a simplex in $\mathbb{S}(n, 1)$ by Theorem 1. The simplex X^*such that $\mathbf{X}$ is the dihedral Gram matrix of X^*, is by Proposition 8 the realization obtained as before of $\Psi(\mathbf{X}) \in C_n^+$. Uniqueness up to isometry follows from Proposition 6, or see [20].

The two other cases can be dealt with in the same fashion, but this requires a more careful analysis of the linear algebra. So here is a more direct argument:

For $\mathbf{X} \in C_n^-$ put $\hat{\mathbf{X}} = \mathbf{X}$ and for $\mathbf{X} \in H_n$ put $\hat{\mathbf{X}} = -\mathbf{X}$. Then in both cases $\hat{\mathbf{X}}$ has index 1, hence:

$$\hat{\mathbf{X}} = \mathbf{Y}^{\mathbf{t}}\mathbf{I}_1\mathbf{Y} = \mathbf{G}_Y, \tag{2.31}$$

[4] e.g. from Theorem 1 or Theorem 2

for some $\mathbf{Y} \in \mathrm{Gl}_{n+1}(\mathbb{R})$, see page 10. Then the set columns of $\mathbf{Y}$, denote this set by X, gives the desired subsets of respectively $\mathbb{M}(n, 1, 1)$ and $\mathbb{M}(n, 0, -1) = \mathbb{H}(n, -1)$ such that $\mathbf{C}_\kappa(X) = \mathbf{X}$, c.f. Remark 5, with uniqueness up to isometry as before.

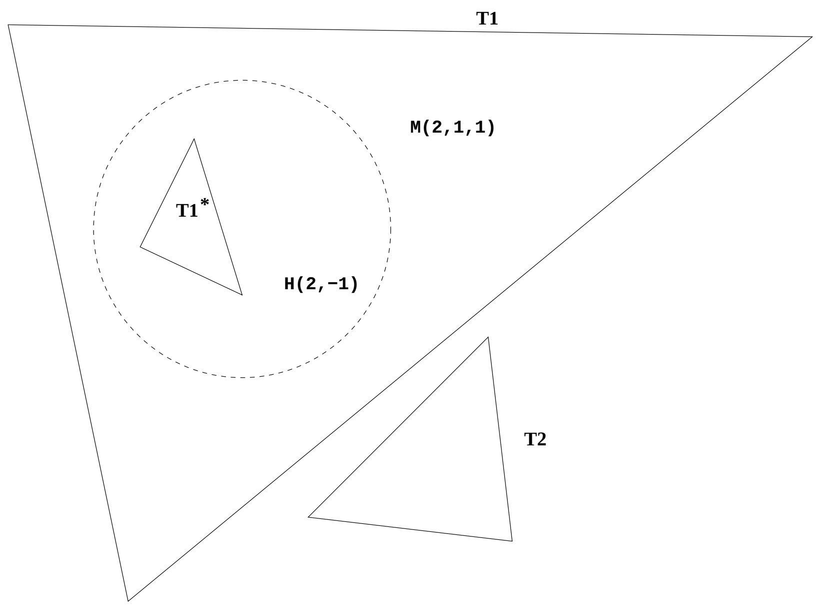
For $\mathbf{X} \in C_n^-$ defining X^* as the realization of $\Psi(\mathbf{X}) \in H_n$, as directly above, gives by Proposition 8 a hyperbolic simplex with dihedral Gram matrix $\mathbf{X}$. ☐

We see that it would be sensible to define the dihedral Gram matrix of a simplex $X \subset \mathbb{M}(n, 1, 1)$, with $\mathbf{C}_\kappa(X) \in C_n^-$, to be the $\mathbf{C}_\kappa$-matrix of the dual hyperbolic simplex, i.e. $\Psi(\mathbf{C}_\kappa(X))$. Then the dihedral angles would be in $\mathbf{i}\mathbb{R}_+$.

The Lorentzian space $\mathbb{M}(n, 1, 1)$ is called the *de-Sitter sphere*. Not all simplices in $\mathbb{M}(n, 1, 1)$ are dual to hyperbolic simplices, this is in fact the case only for those which have $\mathbf{C}_\kappa$-matrix in C_n^- (all cofactors positive). Since a principal minor of $\mathbf{C}_\kappa(X) \in C_n^-$ is positive definite (by definition) we see that every codimension 1 face is in fact a spherical simplex in a spacelike hypersurface of $\mathbb{M}(n, 1, 1)$, which is isometric to $\mathbb{M}(n-1, 0, 1) = \mathbb{S}(n-1, 1)$. Hence also faces of higher codimension are spherical simplices.

Viewing such a simplex $X \subset \mathbb{M} = \mathbb{M}(n, 1, 1)$, pasted together of spherical simplices, as a closed chain complex, X defines a homology class. It can be shown, that a simplex X with spacelike faces is dual to a hyperbolic simplex iff this homology class is nontrivial (X encloses the $\mathbb{S}^{n-1}$-factor, see the sketch).

Figure 2.3: Projective model of $\mathbb{H}(2, -1)$ and the upper hemisphere of $\mathbb{M}(2, 1, 1)$. The triangle **T1** encloses the hyperbolic space and has a corresponding dual triangle $\mathbf{T1}^* \subset \mathbb{H}(2, -1)$, while the triangle **T2** is not dual to a hyperbolic triangle.



What the map Ψ does in both the

sphere$\leftrightarrow$*sphere*, and the *de-Sitter sphere*$\leftrightarrow$*hyperbolic space* duality

is from the point of view of the ambient $\mathbb{R}^{n+1}_\nu$:

$\mathbf{C}_\kappa(X)$ is the Gram matrix for a set of position vectors $\tilde{X}$ which form a basis for $\mathbb{R}^{n+1}_\nu$, i.e. $\mathbf{C}_\kappa(X) = \mathbf{X^t I_\nu X}$, where $\tilde{X}$ are the columns of $\mathbf{X}$ and ν is either 0 (the sphere) or 1. Then take the dual basis of $\tilde{X}$, which is given by the columns of $\mathbf{I}_\nu\mathbf{X}^{-1,t}$. Take the Gram matrix of this dual basis $\tilde{X}^*$, and finally normalize it, by multiplying from right and left with $\mathbf{N}$, so that diagonal entries become 1.

The duality, as formulated here for simplices, is nothing more than taking dual basis with respect to the scalar product $\langle\cdot,\cdot\rangle$. This interchanges edge lengths and dihedral angles of a simplex. However the importance of the formulation via $\mathbf{C}_\kappa$-matrices is that:

The duality operation makes sense without reference to any ambient space!

Hence it could be defined, and perhaps be interesting, in other contexts...

Finally let's give a distance formulation:

Definition 13. For $\kappa \in \mathbb{R}\setminus\{0\}$ and $X = \{p_1, \dots, p_{n+1}\}$ the vertices of a simplex in $\mathbb{M}(n,\kappa)$ with exterior dihedral angles $[\theta_{ij}]$, define a dual distance space

$$X^* = \{p_1^*, \dots, p_{n+1}^*\} \text{ with distance matrix}$$

$$\mathbf{D}_{X^*} := \Big[\frac{1}{\sqrt{|\kappa|}}\theta_{ij}\Big] \in \mathcal{D}_{n+1}(\mathbb{R}_+)$$

Corollary 1. *Let $\kappa \in \mathbb{R}\setminus\{0\}$ and let X be the vertex set of a simplex in $\mathbb{M}(n,\kappa)$ then:*

$$X^* \overset{isom}{\hookrightarrow} \mathbb{S}(n,\kappa) \textit{ for } \kappa > 0$$

$$X^* \overset{isom}{\hookrightarrow} \mathbb{M}(n,1,|\kappa|) \textit{ and } \mathbf{i}X^* \overset{isom}{\hookrightarrow} \mathbb{M}(n,n-1,\kappa) \textit{ for } \kappa < 0$$

In every case X^* is a metric space.

Proof. In the case $\kappa > 0$ it follows from the proposition above (by scaling), that X^* is realizable in $\mathbb{S}(n,\kappa)$, and is thus a metric space.

In the case $\kappa < 0$ (again by scaling) X^* is realizable in $\mathbb{M}(1,1,|\kappa|)$. And (by the discussion above) all proper faces $Y \subset X^*$ are simplices in $\mathbb{S}(|Y|-1,\kappa)$. So if $n+1 \geq 4$, every 3 points lie in a sphere, hence satisfy the triangle inequality.

Using the Gauss-Bonnet formula it is easily established, that also for 3 points, X^* is a metric space.

Multiplying the metric of $\mathbb{M}(n,1,|\kappa|)$ with -1, we obtain the realization $\mathbf{i}X^* \overset{isom}{\hookrightarrow} \mathbb{M}(n,n-1,\kappa)$. $\square$

Remark 8. For a spherical simplex $X \subset \mathbb{S}(n,\kappa)$, the dual X^* is again a simplex in $\mathbb{S}(n,\kappa)$. There is also a distance characterization of the duality, cf. [29].

$$\Delta(X^*) \underset{isom}{\cong} \{p \in \mathbb{S}(n,\kappa) | \, d(p, \Delta(X)) \geq \frac{\pi}{2\sqrt{\kappa}}\}$$

The convex hull of X^*, $\Delta(X^*)$ is called the *polar dual* of $\Delta(X)$ while the closure of the complement $\mathbb{S}(n,\kappa) \setminus \big(\Delta(X^*) \cup \sigma_A(\Delta(X^*))\big)$ is called the *complementary dual*. Here σ_A is the antipodal isometry. This set can be identified with the set of oriented hypersurfaces intersecting $\Delta(X)$. See [31] and [24].

Examples

The connection between the algebra of the $\mathbf{C}_\kappa(X)$-matrix and the geometry of the simplex spanned by X provides us with a geometric interpretation of various formulas from linear algebra. This establishes the theory as a powerful tool to treat the geometry of simplices, and thus polytopes, in high dimensional spaces.

Example 3. For example in the Riemannian cases, and $\kappa \neq 0$, expanding $\det(\mathbf{C}_\kappa(X))$ after row i, we get:

$$\det(\mathbf{C}_\kappa(X)) = c_{ii} + \sum_{j \neq i} c_{ij} \mathbf{c}_\kappa(d_{ij}),$$

where $[c_{ij}] = \operatorname{cof}(\mathbf{C}_\kappa(X))$. Using Proposition 8 this becomes:

$$\det(\mathbf{C}_\kappa(X)) = c_{ii} + \sum_{j \neq i} \cos(\theta_{ij}) \sqrt{c_{ii}} \sqrt{c_{jj}} \mathbf{c}_\kappa(d_{ij})$$

Dividing by $c_{ii} = \det(\mathbf{C}_\kappa(X_i))$ and using (2.20), we arrive at:

$$\mathbf{s}_\kappa(h_i)^2 = 1 + \sum_{j \neq i} \cos(\theta_{ij}) \frac{\mathbf{s}_\kappa(h_i)}{\mathbf{s}_\kappa(h_j)} \mathbf{c}_\kappa(d_{ij}), \tag{2.32}$$

where h_i is the altitude from p_i onto S_{X_i}. From this we can e.g. find a relation between the dihedral angles θ, altitudes h and edge lengths l of a regular simplex $X \subset \mathbb{M}(n,\kappa)$:

$$\mathbf{s}_\kappa(h)^2 = 1 + n \cos(\theta) \mathbf{c}_\kappa(l) \tag{2.33}$$

(Note that for $\kappa < 0$, $\mathbf{s}_\kappa(h)^2$ is negative by the definition of $\mathbf{s}_\kappa$, (1.6)). For $\kappa \neq 0$ the dual simplex X^*, which by symmetry is also regular, has edge lengths $l^* = \frac{\theta}{\sqrt{|\kappa|}}$, hence we obtain the symmetric (duality invariant) expression:

$$\mathbf{s}_\kappa(h)^2 = 1 + n \mathbf{c}_{|\kappa|}(l^*) \mathbf{c}_\kappa(l) = \mathbf{s}_{|\kappa|}(h^*)^2 \tag{2.34}$$

We see that the regular simplex in $\mathbb{S}(n,\kappa)$ with $l = \frac{\pi}{2\sqrt{\kappa}}$ is *self dual*[5].

[5] which is almost *self* evident…

Example 4. From (2.28) we deduce

$$\det(\mathbf{C}_\kappa(X^*)) = \det(\mathbf{C}_\kappa(X))^n \prod_{i=1}^{n+1} \det(\mathbf{C}_\kappa(X_i))^{-1},$$

But then using Theorem 2 and (2.20), we see:

$$\det(\mathbf{C}_\kappa(X^*)) = \prod_{i=2}^{n+1} \mathbf{s}_\kappa(h^*_{<i})^2 = \det(\mathbf{C}_\kappa(X)^{-1}) \prod_{j=1}^{n+1} \mathbf{s}_\kappa(h_j)^2$$

It is possible to produce lots of relations like this…

Example 5. The determinant of $\mathbf{C}_\kappa(X)$ is just one of the invariants appearing in the characteristic polynomial:

$$\chi(\lambda) = \det(\mathbf{C}_\kappa(X) - \lambda\mathbf{I}) = \sum_{i=0}^{n+1} a_i \lambda^i \tag{2.35}$$

Here

$$a_i = (-1)^i \Sigma_{|X|-i}(\lambda_1, \ldots, \lambda_n) = (-1)^i \sum_{|I|=i} |\mathbf{C}_\kappa(X)_I|,$$

where $\Sigma_{|X|-i}$ is the $(|X| - i)$'th elementary symmetric polynomial, which is evaluated in the eigenvalues $\lambda_1, \ldots, \lambda_n$; the last sum is over all principal minors obtained by deleting i rows and columns. Written differently we have:

$$a_i = (-1)^i \sum_{|X\setminus Y|=i} \det(\mathbf{C}_\kappa(Y)) \tag{2.36}$$

a sum over all faces $Y \subseteq X$ of codimension i. Then one has, for example:

$$-\frac{a_1}{a_0} = \mathrm{trace}(\mathbf{C}_\kappa(X)^{-1}) = \sum_{i=1}^{n+1} \frac{1}{\lambda_i} = \sum_{i=1}^{n+1} \frac{1}{\mathbf{s}_\kappa(h_i)^2}, \tag{2.37}$$

where the λ_i's are the eigenvalues of $\mathbf{C}_\kappa(X)$. The last equality follows using (2.20) on $-\frac{a_1}{a_0}$.

Example 6. Let $\gamma(t) = X_t$ be a curve of simplices in $\mathbb{M}(n, \kappa)$, $n \geq 2$. We may consider such a curve as $n+1$ vertex curves, i.e. $\gamma : I \to \mathbb{M} \times \mathbb{M} \times \cdots \times \mathbb{M}$, with $n+1$ factors, such that the vertices of X_t, which are the coordinates of γ_t, are in general position.

The classical *Schläfli differential equality* gives a formula for the derivative of the volume of the convex hull $\Delta(X_t)$ (see [20] or [31]):

$$\frac{d}{dt}\,\mathrm{vol}(\Delta(X_t)) = \frac{-1}{\kappa(n-1)} \sum_{i<j} \mathrm{vol}\left(\Delta(X_{ij})(t)\right) \frac{d}{dt}\theta_{ij}, \tag{2.38}$$

a sum over all codimension 2 faces X_{ij}. The non standard -1 factor is due to the fact that we use *exterior* dihedral angles $\theta_{ij} = \pi -$interior angles.

With the notation of Definition 13, we can write this in the appealing manner:

$$\frac{d}{dt}\operatorname{vol}(\Delta(X_t)) = \frac{-\operatorname{sign}(\kappa)}{2(n-1)}\operatorname{trace}(\mathbf{V}_t \frac{d}{dt}\mathbf{D}_{X_t^*}), \tag{2.39}$$

where the entries of $\mathbf{V}_t = [V_{ij}(t)]$ are $V_{ij}(t) := \frac{1}{\sqrt{|\kappa|}}\operatorname{vol}(\Delta(X_{ij})(t))$ and the factor of $\frac{1}{2}$ is because we get all terms twice in the trace. This seems to suggest a determinant formula for the volume of a simplex, using the duality!

Example 7 (Volume of a n-simplex). Using the theory developed, we can obtain a closed formula for the volume of a regular n-dimensional simplex in any curvature.

The $\mathbf{C}_\kappa(X)$ matrix of a regular simplex has one's along the diagonal and off diagonal entries equal to $\mathbf{c}_\kappa(l)$, where l is the edge lengths. Now we will fix the curvature to be ± 1 and consider $t = \sqrt{|\kappa|}$ as the edge lengths; this is geometrically the same as considering a simplex with edge lengths 1 in curvature κ.

From Proposition 8 we obtain using that indices are symmetric:

$$\cos(\theta_{ij}) = \frac{c_{ij}}{\sqrt{c_{ii}}\sqrt{c_{jj}}} = \frac{c_{12}}{c_{11}} = \frac{c_{12}}{\det(\mathbf{C}_\kappa(X_1))}, \tag{2.40}$$

We already have a formula for $|\mathbf{C}_\kappa(X_1)|$, since X_1 is a regular $(n-1)$-simplex. Likewise we can easily find a formula for the other minor. We get:

$$\cos(\theta) = \frac{-\mathbf{c}_\kappa(1)(1-\mathbf{c}_\kappa(1))^{n-1}}{\big((n-1)\mathbf{c}_\kappa(1)+1\big)(1-\mathbf{c}_\kappa(1))^{n-1}} = \frac{-\mathbf{c}_\kappa(1)}{(n-1)\mathbf{c}_\kappa(1)+1} := \lambda(\kappa) \tag{2.41}$$

So $\cos(\theta)$ is a rational function evaluated in $\mathbf{c}_\kappa(1)$. We can obtain nicer expressions for this, however we only want to point out the possibility of doing so. Then we obtain θ as $\operatorname{Arccos}(\lambda(\kappa))$. Finally integrate the Schläfli differential equality, cf. Example 6 to obtain:

$$\begin{aligned}\operatorname{vol}(X_\kappa) = -\frac{(n+1)n}{(n-1)2}\operatorname{sign}(\kappa)\int_0^t t\frac{d}{dt}\operatorname{Arccos}\big(\lambda(\kappa)\big)dt = \\ -\frac{(n+1)n}{(n-1)2}\operatorname{sign}(\kappa)\bigg(\operatorname{Arccos}(\lambda(\kappa))\sqrt{|\kappa|} - \int_0^t \operatorname{Arccos}(\lambda(\kappa))dt\bigg),\end{aligned} \tag{2.42}$$

where we use $t = |\sqrt{\kappa}|$ as a parameter in differentiations and integrations. There is a factor of $\frac{(n+1)n}{(n-1)2}$ in front because we sum over the $\binom{n+1}{2}$ codimension 2 faces and then divide by $n-1$.

So this is the volume of a n-dimensional simplex with edge lengths $\sqrt{|\kappa|}$ in curvature ± 1. To obtain a formula for a simplex with edge lengths 1 in curvature κ, divide the above expression by $\sqrt{|\kappa|^n}$.

In the hyperbolic case, curvature -1, taking the limit of the formula above, as $|\kappa| \to \infty$, gives the volume of an *ideal* simplex. This is the unique simplex in $\mathbb{H}(n,-1)$ of maximal volume, compare [11],[20]. A computation with *Maple* gives in the case $n = 3$: $V_3^{max} \cong 1.01494\ldots$ in accordance with [20] p. 200.

2.5 Duality via Half Spaces and Distance functions

Here we shall give another description of the duality for the Riemannian space forms from an intrinsic and more "global" viewpoint. The description is very loose and proofs are omitted. As we shall see later, most of the ideas has translations in a quite different setting, namely for *weighted trees*, another important class of metric spaces.

Half Spaces Let $\mathbb{M}^n$ be one of the Riemannian space forms $\mathbb{M}(n, \kappa)$. We use d to denote $d_{\mathbb{C}}$, which here is the usual Riemannian distance. Let $S \subset \mathbb{M}^n$ be an oriented hypersurface, i.e. S is totally geodesic[6], isometric to $\mathbb{M}^{n-1}$ and has a smooth normal vector field $\mathbf{n}$.

The (closed) *half space* $H \subset \mathbb{M}$ determined by S, is the subset of $\mathbb{M}$ such that $S = \partial H$ and $p \in H$ iff $p \in S$ or $df(\mathbf{n}) < 0$, where $f = d(\cdot, p)$ is the distance from p, which is smooth away from p and the antipode of p if $\kappa > 0$. We have defined H such that $\mathbf{n}$ "points into" H. Then the set of oriented hypersurfaces is identified with the set of half spaces , and this set form a double cover of the set of hypersurfaces by $H \mapsto \partial H$.

Note that by the symmetry of the space forms an oriented hypersurface S is determined by *a single vector* in $TS^{\perp}$. In the ambient space picture, any vector $v \in T_pS^{\perp}$ is parallel to the normal vector $\tilde{v}$ to the linear hyperplane $\tilde{S}$ such that $S = \mathbb{M} \cap \tilde{S}$.

Distance Functions on Riemannian Manifolds A Lipschitz continuous function on a Riemannian manifold M is differentiable almost everywhere (with respect to volume measure); this follows from Rademachers Theorem, c.f. [6]. Then for a Lipschitz function f, $df \in T^*M$ is well defined almost everywhere. Define the norm of df as usual at a differentiable point $p \in M$:

$$\|df_p\| := \sup\{|df_p(v)| \mid v \in T_vM, \|v\| = 1\} \tag{2.43}$$

We could also define the *generalized differential*, where f is not smooth, as in [6].

Then Define a *distance function* on a Riemannian manifold M as a Lipschitz continuous function $f : M \to \mathbb{R}$, with Lipschitz constant 1 and $\|df\| = 1$ where f is differentiable. Note that with this convention also $-f$ is a distance function if f is! We could have defined this more explicitly for the space forms...

Define $\mathcal{D}f(M)$ as the set of distance functions on M. Note that $f = d(\cdot, p)$, the distance from $p \in M$ is smooth everywhere except from $p \cup C_p$, where C_p is the *cut locus* of p (see e.g. [5]). Also $\|df\| = 1$ on $M \setminus (p \cup C_p)$.

We then have an injection: $M \hookrightarrow \mathcal{D}f(M)$ defined as $p \mapsto d(\cdot, p)$.

Definition 14. For $\mathbb{M} = \mathbb{M}(n, \kappa)$ define $\mathbb{M}^*$ as the set of half spaces of $\mathbb{M}$, and define $\mathbb{M}^{**}$ as the subset of distance functions:

$$M^{**} := \{\pm d(\cdot, p) | \, p \in M\} \cup \Big(\mathcal{D}f(\mathbb{M}) \cap \mathbb{C}^{\infty}(M, \mathbb{R})\Big) / \sim, \tag{2.44}$$

[6]and connected for $\mathbb{M}^n \neq \mathbb{S}(1, \kappa)$.

where $f \sim f + c$ for $c \in \mathbb{R}$.

For a convex subset $V \subseteq \mathbb{M}$ define the complementary dual $V^* \subset \mathbb{M}^*$ as the set of half spaces H such that $V \cap \partial H \neq \emptyset$.

Remark 9. A note of warning: For $\kappa \neq 0$ and a finite vertex set $X \subset \mathbb{M}(n, \kappa)$ spanning a simplex, we have defined a (Gram matrix) dual simplex X^*, which we think of as a finite subset in either $\mathbb{S}(n, \kappa)$ or $\mathbb{M}(n, 1, |\kappa|)$. This is closely related to the complementary dual defined above. The convex hull[7] of X^* is what is usually called the *polar dual,* while the complementary dual of $\Delta(X)$, as defined above, can be identified with the closure of the complement of $\Delta(X^*) \cup \sigma_A(\Delta(X^*))$. Here σ_A is the antipodal isometry. For more details see [31], where the complementary dual is only "half" of the complementary dual defined above: it is defined as the set of hypersurfaces intersecting V, while we use *oriented hypersurfaces*.

So we restrict ourselves to $\pm$-distance functions from points and smooth distance functions, which then by definition cannot have any critical points (in the usual sense). We then again have an injection of $\mathbb{M}$ into the space $\mathbb{M}^{**}$, $\mathbb{M} \hookrightarrow \mathbb{M}^{**}$, $p \mapsto d(\cdot, p)$. Call $\mathbb{M}$ reflexive if $\mathbb{M} = \mathbb{M}^{**}$. It is clear that the spheres are reflexive. But for $\kappa \leq 0$ the inclusion $\mathbb{M} \hookrightarrow \mathbb{M}^{**}$ is strict; there are distance functions corresponding to “points outside” $\mathbb{M}$. Hence we can think of $\mathbb{M}^{**}$ as a kind of *completion* of $\mathbb{M}$.

In a sense $\mathbb{M}^{**}$ should be considered as the set of half spaces of $\mathbb{M}^*$. For $f \in \mathbb{M}^{**}$ define

$$H(f) := \{(S, \mathbf{n}) \in \mathbb{M}^* \mid df(\mathbf{n}) \leq 0 \text{ almost everywhere on } S\}.$$

Then $H(f)$ contains "half "of the half spaces of $\mathbb{M}$.

We will not go into further details with this here, but just mention that for $\kappa = 0$ we can identify the smooth distance functions with distances from the sphere at infinity, giving rise to a geodesic foliation of $\mathbb{M}$ into parallel lines. And for $\kappa < 0$, we have two types of smooth distance functions: distances from the sphere at infinity and distances from $\mathbb{M}(n, 1, |\kappa|)$. Each type of function giving rise to a type of geodesic foliation via the integral curves of ∇f. For $p \in \mathbb{H}(n, \kappa)$ the distance function $-d(\cdot, p)$ corresponds to a point in the lower embedding of $\mathbb{H}(n, \kappa)$.

For $p \in \mathbb{M}$ define $\overset{**}{p}$ as $H(d(\cdot, p))$: the set of half spaces containing p. We may think of the complementary dual $p^* \subset \mathbb{M}^*$ as forming the boundary of the half space $\overset{**}{p}$.

Acting by Isometries The isometry group $\mathrm{Isom}(\mathbb{M}^n)$ acts transitively on $\mathbb{M}^*$, and the isotropy group fixing a half space H, or equivalently the oriented hypersurface ∂H, can be identified with $\mathrm{Isom}(\partial H) = \mathrm{Isom}(\mathbb{M}^{n-1})$. Hence we have an identification, which we can define to be a diffeomorphism.

$$\mathbb{M}^* \cong \mathrm{Isom}(\mathbb{M}^n)/\,\mathrm{Isom}(\mathbb{M}^{n-1}) \tag{2.45}$$

[7] which makes sense in $\mathbb{M}(n, 1, |\kappa|)$ also

In all three geometries $\mathrm{Isom}(\mathbb{M}^n)$ is unimodular and has a Haar measure (c.f. [27], [22] 6.6) which then via the identification above gives an $\mathrm{Isom}(\mathbb{M}^n)$ invariant measure μ on $\mathbb{M}^*$.

Let $A \triangle B = A \cup B \setminus A \cap B$ denote the symmetric difference between two subsets A, B of some larger set. Using that $\mathbb{M}$ is 2-point homogeneous it can be seen that $\mu(\overset{**}{p} \triangle \overset{**}{q})$ depends only on $d(p, q)$. In fact there is a positive constant k s.t. $\mu(\overset{**}{p} \triangle \overset{**}{q}) = kd(p, q)$. We shall not prove this here, but refer to [27] for the proof in the case $\kappa < 0$; the other cases are similar. We can then normalize μ such that $\mu(\overset{**}{p} \triangle \overset{**}{q}) = d(p, q)$, which will be assumed in the following.

For a convex set $V \subset \mathbb{M}$, the measure of V^* turns out to be interesting:

Definition 15. For a convex subset $V \subset \mathbb{M}$, $\mu(V^*)$ is called the complementary dual volume of V.

We see from the preceding discussion that the dual volume of V is the measure of the set of oriented hypersurfaces intersecting V, or 2 times the measure of the hypersurfaces intersecting V.

Extrinsic Description Let us see how the "half-space formulation" of the duality works via the linear geometry of the ambient semi-Euclidean space.

For $\kappa \neq 0$ we have $\mathbb{M} = \mathbb{M}(n, \kappa) \subset \mathbb{R}^{n+1}_\nu$ with $\nu = 0$ if $\kappa > 0$ and $\nu = 1$ if $\kappa < 0$. For $\kappa = 0$, i.e. $\mathbb{M} = \mathbb{R}^n$, we will consider $\mathbb{R}^n \overset{isom}{\hookrightarrow} \mathbb{R}^{n+1}$, embedded as the affine hyperplane $x_{n+1} = 1$. Then the discussion in all three cases is unified:

Every half space $H \subset \mathbb{M}$ is simply the intersection with $\mathbb{M}$ of a half space $\tilde{H} \subset \mathbb{R}^{n+1}_\nu$ determined by an oriented linear n-dimensional subspace $\partial \tilde{H} \subset \mathbb{R}^{n+1}_\nu$. $\partial \tilde{H}$ intersects $\mathbb{M}$ in the hypersurface $\partial H \subset \mathbb{M}$ which determines the half space H via the orientation inherited from $\partial \tilde{H}$. The orientation corresponds to a unique normal vector $n \in \partial \tilde{H}^\perp$ chosen such that $|\langle n, n \rangle| = \frac{1}{\kappa}$ if $\kappa \neq 0$ and $\langle n, n \rangle = 1$ if $\kappa = 0$. In this way $\mathbb{M}^*$ is identified with a subset of $\mathbb{R}^{n+1}_\nu$.

For $\mathbb{M} = \mathbb{S}(n, \kappa) \subset \mathbb{R}^{n+1}$ it is clear that $\mathbb{M}^*$ is simply $\mathbb{S}(n, \kappa)$ again and $\overset{**}{p}$ can be identified as the half space H which contains p as the north pole, i.e. ∂H is the intersection of $\mathbb{S}(n, \kappa)$ with $\tilde{p}^\perp \subset \mathbb{R}^{n+1}$.

A linear subspace $\partial \tilde{H}$ in $\mathbb{R}^{n+1}_1$ intersects $\mathbb{M} = \mathbb{H}(n, \kappa) \subset \mathbb{R}^{n+1}_1$ iff $\partial \tilde{H}$ is non degenerate of index 1, which is the case iff the normal is spacelike. We see that $\mathbb{M}^*$ is $\mathbb{M}(n, 1, |\kappa|)$, the de Sitter sphere. $\overset{**}{p}$ is identified with the half space H of $\mathbb{M}(n, 1, |\kappa|)$, such that $\partial H = \mathbb{M}(n, 1, |\kappa|) \cap \tilde{p}^\perp \subset \mathbb{R}^{n+1}_1$ and such that the intersection with $\mathbb{M}(n, 1, |\kappa|)_+$, the upper hemisphere, is unbounded.

For $\mathbb{M} = \mathbb{R}^n$, $\mathbb{M}^*$ is identified with $\mathbb{S}(n, 1)$ minus two antipodal points.

Then we can put a measure μ on $\mathbb{M}^*$ via this identification. For $\kappa \neq 0$ we simply use the semi-Riemannian volume form c.f. [21] on the corresponding dual[8].

[8] In the case of $\mathbb{R}^n$ the description is slightly more involved...

In fact we get the same measure as in the isometry group construction, modulo a positive constant. Summarizing we have:

Theorem 3. *Let* $\mathbb{M}$ *be one of the Riemannian space forms* $\mathbb{M}(n, \kappa)$. *There is a measure on* $\mathbb{M}^*$ *such that the map* $p \mapsto \overset{**}{p}$ *is an isometry:*

$$\forall p, q \in \mathbb{M} : \ d(p, q) = \mu(\overset{**}{p} \triangle \overset{**}{q}), \tag{2.46}$$

where $\overset{**}{p} = H(d(\cdot, p))$, *the half spaces containing* p.

Remark 10. It makes sense to use the word isometry, since for a measure space $(\Omega, \mathcal{A}, \mu)$, $d_\mu = \mu(A \triangle B)$ is a semimetric on the set of measurable subsets $\mathcal{A}$. See [7].

2.6 Graphs

Here we will discuss a duality construction for graphs similar to the one given above. Since we shall also be concerned with graphs later, we will first recapitulate some fundamental concepts of this subject. We refer to [7] for more details.

$G = (V, E, w)$ will denote a simple, undirected weighted graph. Here V is the set of *vertices* and E is the set of edges, which we consider as a subset of the set of unordered pairs of V, such that $e = uv \in E$ implies $u \neq v$ (no loops) . If two vertices u, v is contained in a common edge they are called adjacent. The set of *neighbors* of a vertex $v \in V$ is the set of vertices adjacent to v, denote this set by $N(v) := \{u \in V | uv \in E\}$. The *degree* of a vertex $v \in V$ is the cardinality of the set $N(v)$, the number of edges incident to v. This is denoted $\deg(v)$ and is always assumed *finite*.

The last element of the triple (V, E, w) is the weight function $w : E \to \mathbb{R}^*_+$, which associates a positive weight or *length* to each edge. The weight function extends to a measure on E, by summing edges.

We then get a natural induced metric on V by setting

$$d_w(v_1, v_2) := \inf\{l(\gamma) := \sum_{e \in \gamma'} w(e)\}, \tag{2.47}$$

where the infimum is taken over all *paths* γ joining v_1 and v_2. Here a path joining v_1 and v_2 is a sequence of vertices $\gamma : v_1 = u_1, u_2, \ldots, u_n = v_2$ such that $u_i u_{i+1} \in E$ (γ' denotes the associated sequence of edges). We also allow one point paths $\gamma = v \in V$, and put the length of such a path equal to zero so that $d(v, v) = 0$. The *combinatorial distance function* on V , $d_c : V \times V \to \mathbb{N}_0$ is obtained by defining $w(e) = 1, \forall e \in E$.

A graph is connected if all vertices are joined by a path. A *tree* is a connected graph which contains no circuits, i.e. there is no sequence $v = v_1, v_2, \ldots, v_n = v$ such that $n > 2$, $v_i v_{i+1} \in E$ and $v_i \neq v_j$ for $2 \leq i < j \leq n$.

Geometrization Geometrizing a weighted graph consist of the following, c.f. [19]: consider the graph G as a locally finite 1-dimensional simplicial complex, which we denote by $\tilde{G}$. The 0-simplices of $\tilde{G}$ corresponds to the vertices V; write $\tilde{v}$ for v considered as 0-simplex. The 1-simplices of $\tilde{G}$ corresponds to the edge set E, in the obvious way that an edge $e = uv$ is identified with a 1-simplex $\tilde{e}$, having boundary points $\tilde{u}, \tilde{v}$. Then we give each 1-simplex a metric such that $\tilde{e} \underset{isom}{\cong} [0, w(e)]$.

The metric (i.e. distance) d_w is then extended to a length space metric on $\tilde{G}$, containing the graph vertex set V as an isometric subspace. By assumption of finiteness of $\deg(v)$, for all $v \in V$, this space is locally compact, complete and geodesic.

We may then rephrase the condition that a graph is a tree as: *the geometrization $\tilde{G}$ is simply connected.*

Half space duality for Graphs

Now we shall get to the promised duality discussion. We could just as well formulate the construction for the geometrization of a graph, but here we choose to work with the discrete graph in itself, just to see that things work out nicely in this setting.

Oriented hypersurfaces Let $G = (V, E, w)$ be a weighted, connected graph. Define the tangent space at $v \in V$ as

$$T_v G := \bigcup_{u \in N(v)} uv, \quad \text{and the tangent bundle } TG := \bigsqcup_{v \in V} T_v G.$$

An element of TG can then be considered as a pair $\mathbf{v} = (v, uv)$, consisting of a vertex v and en edge incident to v. We will think of the edge set E as the set of *hypersurfaces* and thus of TG as the set of oriented hypersurfaces, which forms a double cover of E. The weight function w measure on E extends to TG.

Distance Functions For a function on $f : V \to \mathbb{R}$ we get an associated function on each tangent space $T_v G$, $df_v : TG \to \mathbb{R}$ defined as:

$$df_v(\mathbf{v}) = f(u) - f(v), \quad \text{for } \mathbf{v} = (v, uv) \in T_v G \tag{2.48}$$

We will think of df_v as the differential of f at v. Define the norm of df_v as:

$$\|df_v\| := \max(|df(\mathbf{v})| \mid \mathbf{v} \in T_v G\} \tag{2.49}$$

Then we can define the set of *combinatorial distance functions*:

$$\mathcal{D}\not{f}_c(G) = \{f : V \to \mathbb{Z} |\ \|df_v\| = 1\, \forall v \in V\} \tag{2.50}$$

It is then easy to see that we, as in the case of Riemannian manifolds, have an injection $V \hookrightarrow \mathcal{D}\not{f}_c(G)$ by mapping $v \mapsto d_c(\cdot, v)$, the combinatorial distance from v.

Now given a function $f \in \mathcal{D}\!\!\not{f}_c(G)$ define the set $H(f) := \{\mathbf{v} \in TG | \, df(\mathbf{v}) \leq 0\}$. Given two functions in $f, g \in \mathcal{D}\!\!\not{f}_c(G)$ we can define the distance between them as:

$$\overset{**}{d}(f, g) := \frac{1}{2} w(H(f) \triangle H(g)), \tag{2.51}$$

where the weight function is extended to a measure on TG. In general this might not be very useful, but at least we have:

Proposition 10. *If* $T = (V, E, w)$ *is a weighted tree, then*

$$(V, d_w) \overset{isom}{\hookrightarrow} (\mathcal{D}\!\!\not{f}_c(T), \overset{**}{d})$$

by the mapping $v \mapsto \overset{**}{v} := H(d_c(\cdot, v))$*, i.e.:*

$$d_w(u, v) = \frac{1}{2} w(\overset{**}{u} \triangle \overset{**}{v}) \tag{2.52}$$

Proof. Simply observe that there is a unique path γ between two vertices $u, v \in V$, denote by $-\gamma$ the reversed path that goes from v to u. On this path the differentials of $f = d_c(\cdot, v)$ and $g = d_c(\cdot, u)$ will have opposite sign, while for all tangent vectors not tangent to γ or $-\gamma$ they agree. Hence the symmetric difference $H(f) \triangle H(g)$, consists of all tangent vectors to γ and $-\gamma$. The result follows, remembering the factor $\frac{1}{2}$ in the definition of $\overset{**}{d}$. □

This is very similar to the construction in the space forms. We can also think of the set $\overset{**}{v}$ as the *half spaces containing* v in the case of a tree where every "hypersurface", i.e. an edge, divides T into two disjoint parts. This is really what makes the construction work in both the $\mathbb{M}(n, \kappa)$ and the weighted tree cases.

2.7 The Isometric Embedding Problem

By Theorem 1 every $\mathbb{C}_\kappa$-distance space X is realizable as a subset of some $\mathbb{M}(n, \nu, \kappa)$. Here we shall be particularly interested in *metric spaces*, and the question:

what are the properties of the set of curvatures κ *such that* $X \overset{isom}{\hookrightarrow} \mathbb{M}(n, \kappa)$?

Berestovskij has shown, c.f. [3], that for a metric space X with 4 points, the set of curvatures such that X is realizable in $\mathbb{M}(3, \kappa)$ is an interval, if nonempty. The proof uses in an essential way, that for a nondegenerate isometrically realized triangle in $\mathbb{M}(n, \kappa)$ the distance from a vertex to a "fixed" point on the opposite side depends in a very simple way on the curvature: *it is strictly increasing as a function of this.*

This does not generalize to simplices of higher dimension. First of all, it is not immediately clear how to define a "fixed" point on a face opposite to a vertex. But the *altitude* from a vertex makes good sense, and can be studied via the formula given in Theorem 2. However it turns out that the behavior of the altitude, as a function of curvature, is not so simple for higher dimensional simplices.

The following is a collection of miscellaneous results and observations on what happens for metric spaces withe more than 4 points.

Curves of associated matrices One might think that a finite metric space X, is nothing more than a matrix in $\mathcal{D}_n(\mathbb{R}_+)$, hence a rather "poor" object. But we know from the previous sections that the matrix $\mathbf{C}_\kappa(X)$ has interesting geometric significance, and in fact we have an entire curve of such matrices $\gamma_X : \kappa \mapsto \mathbf{C}_\kappa(X)$ and several derived (analytic) functions like $\kappa \mapsto \det(\mathbf{C}_\kappa(X))$.

There is another useful formulation of realizability, c.f. Theorem 1, using a matrix derived from $\mathbf{C}_\kappa(X)$:

Lemma 7. *Let $X = \{p_0, p_1, \dots, p_{n+1}\}$ be a finite metric space with distance matrix $\mathbf{D} = [d_{ij}] \in \mathcal{D}_{n+2}(\mathbb{R}_+)$. Define the "cosine relation" matrix:*

- *For $\kappa \neq 0$ and $\sqrt{\kappa} \leq \frac{\operatorname{diam}(X)}{\pi}$ (if $\kappa > 0$),*

$$\mathcal{C}_\kappa(X) := [\frac{(\mathbf{c}_\kappa(d_{ij}) - \mathbf{c}_\kappa(d_{0i})\mathbf{c}_\kappa(d_{0j})}{\mathbf{s}_\kappa(d_{0i})\mathbf{s}_\kappa(d_{0j})}] \in \mathcal{N}_n(\mathbb{R}) \tag{2.53}$$

- *For $\kappa = 0$,*

$$\mathcal{C}_0(X) := [\frac{d_{0i}^2 + d_{0j}^2 - d_{ij}^2}{2d_{0i}d_{0j}}] \in \mathcal{N}_n(\mathbb{R}) \tag{2.54}$$

where $i, j \in \{1, \dots, n+1\}$.

Then $X \overset{isom}{\hookrightarrow} \mathbb{M}(m, \nu, \kappa)$ iff $\iota(\mathcal{C}_\kappa(X)) \leq \nu$ and $\rho(\mathcal{C}_\kappa(X)) \leq m - \nu$, hence $X \overset{isom}{\hookrightarrow} \mathbb{M}(m, \kappa)$ iff $\mathcal{C}_\kappa(X)$ is positive semidefinite and $\operatorname{rank}(\mathcal{C}_\kappa(X)) \leq m$.

The lemma is easily derived from Theorem 1, or proven in the same way. It is not necessary that X is a metric space, it works also for $\mathbb{C}_\kappa$-spaces. The entries of $\mathcal{C}_\kappa(X) = [c_{ij}]$ should be thought of as cosines to the "angles" between directions to the other points as seen from p_0, $c_{ij} = \cos(\theta_{ij})$. The criterion of the lemma above is just the criterion for whether this "angle space", Θ, is realizable in $\mathbb{S}(m-1, \nu, 1)$. When X is metric, the angles defined by $\theta_{ij} = \operatorname{Arccos}(c_{ij})$ are real and in $[0, \pi]$.

Then we see that for a metric space, the set of κ's such that $X \overset{isom}{\hookrightarrow} \mathbb{M}(n+1, \kappa)$, realized as a *simplex*, is exactly the set of κ's such that $\mathcal{C}_\kappa(X) \in C_n^+$, where C_n^+ is the set of $\mathbf{C}_\kappa$-matrices of simplices in $\mathbb{S}(n, 1)$, see Proposition 9. The boundary ∂C_n^+ consist of the positive semidefinite, unidiagonal matrices that are not regular. Geometrically a matrix in ∂C_n^+ corresponds to the $\mathbf{C}_\kappa$-matrix of a configuration of $n+1$ points in $\mathbb{S}(n, 1)$, which is not a simplex.

Now for a metric space with $n+2$ points define:

$$\mathcal{K}_X := \{\kappa \in (-\infty, \frac{\pi^2}{\mathrm{diam}(X)^2}]| \mathcal{C}_\kappa(X) \in C_n^+ \cup \partial C_n^+ = \overline{C}_n^+\}, \tag{2.55}$$

Here is a first observation to support the hypothesis that the set of *Riemannian embedding curvatures* is connected:

Observation 3. $\overline{C}_n^+$ is convex (c.f. [20]) hence the curve $\kappa \mapsto \mathcal{C}_\kappa(X)$ is likely to intersect $\overline{C}_n^+$ in a connected set. One approach to establishing that this is always so, would be to show that the curvature of $\kappa \mapsto \mathcal{C}_\kappa(X)$ is small compared to the curvature of the boundary ∂C_n^+.

A boundary points of $\mathcal{K}_X$ corresponds by continuity to a matrix $\mathcal{C}_\kappa(X) \in \partial C_n^+$. For a κ where $\mathcal{C}_\kappa(X) \in \partial C_n^+$, the number

$$|X| - 1 - \mathrm{rank}(\mathcal{C}_\kappa(X)) \tag{2.56}$$

is called the *dimension drop*. We do not know a priori, that for $\mathcal{C}_\kappa(X) \in \partial C_n^+$ we get a boundary point of $\mathcal{K}_X$. This can be phrased as: *does a dimension drop imply that a configuration is rigid to "one side"?* The convexity of $\overline{C}_n^+$ does seem to suggest that this is the generic situation though.

edge lengths

Terminology 2. $X \subset \mathbb{M}(n,\kappa)$ is called convexly independent if $p \notin \Delta(X \setminus \{p\})$ for all $p \in X$; *no point is contained in the convex hull of the other points.* $\kappa = \sup \mathcal{K}_X$ is called a right endpoint and $\kappa = \inf \mathcal{K}_X$ is called a left endpoint. A configuration $X \subset \mathbb{M}(n,\kappa_0)$ is called *rigid* if it is "rigid to both sides" i.e. $\mathcal{K}_X = \{\kappa_0\}$, we could then define the curvature of X as κ_0.

Example 8 (The case $|X| = 4$). Assume that $|X| = 4$, $X \overset{isom}{\hookrightarrow} \mathbb{M}(2,\kappa)$ and that the points are not on a line. Then it follows from [3] that X is rigid if one point is in between two others. κ is a right endpoint if X is convexly dependent or $\kappa > 0$ and the convex hull of X is the entire sphere $\mathbb{S}(n,\kappa)$. And κ is a left endpoint otherwise.

For higher dimensional configurations having a dimension drop it is not so clear how to see geometrically whether X is rigid or κ is a left or right endpoint of $\mathcal{K}_X$. There are examples of convexly independent sets which are right endpoints but not left endpoints, and also examples of rigid convex configurations.

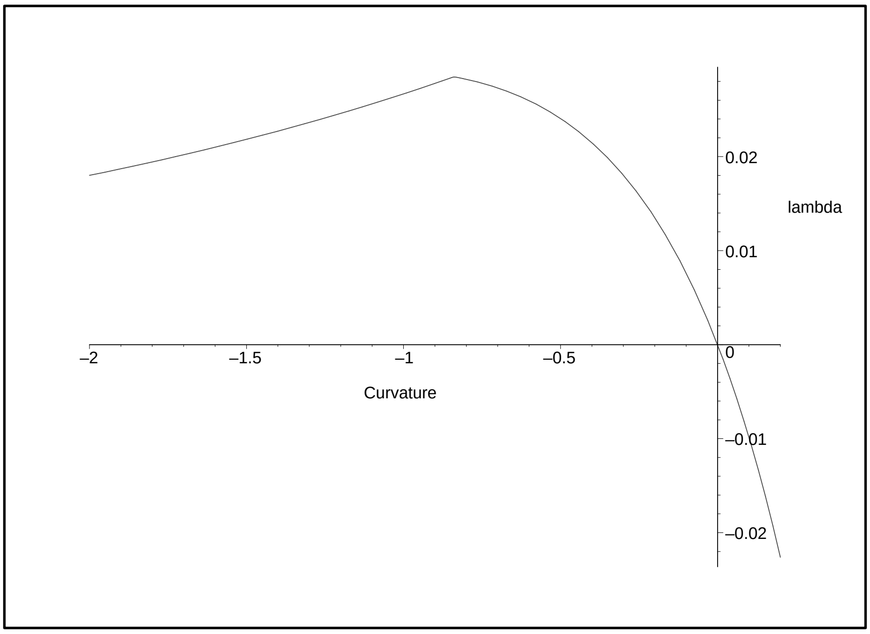
Example 9. Consider a leaf space $X = \{p_1, p_2, p_3, p_4, p_5\}$ (see chapter 3 for terminology) which is the leaf space of a star with $w_1 = w_2 = w_3 = 1$ and $w_4 = w_5 = \frac{1}{6}$. For this space we have $\mathcal{K}_X = (-\infty, 0]$; Figure 2.7 is a plot of the minimal eigenvalue of the cosine relation matrix $\mathcal{C}_\kappa(X)$ (with p_1 as base point).

In the right endpoint $\kappa = 0$ the configuration is realized in $\mathbb{R}^3$ with a dimension drop of 1. Here it consists of a regular triangle T with side lengths 2 and two symmetric points

p_4, p_5 on opposite sides of this triangle, with distance $\frac{1}{3}$ and the geodesic connecting them intersecting T orthogonally through the center of mass. This is a convexly independent configuration.

Perturb X by moving the "axis" connecting p_3 and p_4 towards the boundary of T. This produces a rigid convex configuration before $|p_3 p_4|$ intersects ∂T, as can be checked by e.g. a computer program.

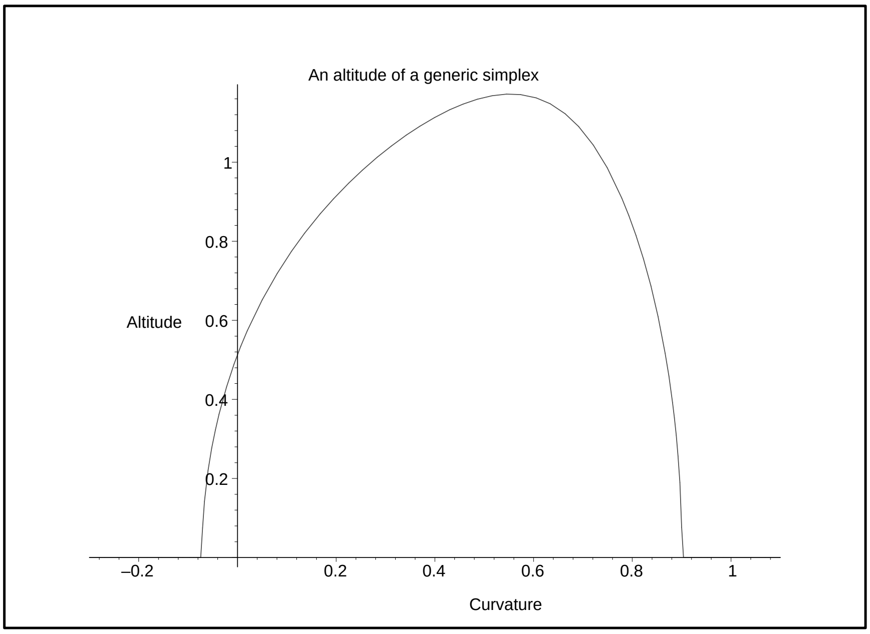
Figure 2.4: A plot of the minimal eigenvalue of $\mathcal{C}_\kappa(X)$, where X is the leaf space discussed in example 9. The configuration collapses with $\kappa = 0$ as a right endpoint. Also note that the graph has a small "bend" corresponding to a curvature where two eigenvalues meet up and interchange roles with respect to being minimal.



From this example we also note that the endpoint $\kappa = 0$ is not determined by the 4-point subsets of X, since these are all non planar and hence realizable in positive curvature. So it is the interplay of all 5 points that determines at least the right endpoint of $\mathcal{K}_X$. Off course the 4-point subsets can always be used to give *bounds* on $\mathcal{K}_X$, since $\mathcal{K}_X \subseteq \mathcal{K}_Y$ for any subset $Y \subset X$. We shall see in chapter 3 that in special cases, which include the space described in the example, the 4-point subsets determine the left endpoint of $\mathcal{K}_X$ completely.

Observation 4. That a configuration X has two symmetric points p, q as in the example above, means that when the configuration collapses with a dimension drop of 1, the altitude from p onto the subspace spanned by $X - \{p, q\}$ is equal to $\frac{1}{2}(d(p, q))$. This is true for those $\kappa \in \mathcal{K}_X$, where $\mathcal{C}_\kappa(X)$ has nullity 1. What we are interested in is whether it is true in general, that we only have at most two such κ's giving a dimension drop. Hence this is related to "concavity" of the altitude as a function of curvature: *does the altitude from a vertex in a simplex onto the opposite face have a unique maximum as a function of curvature?* Examples seem to support this, as is also expected by the convexity of $\overline{C}_n^+$.

Figure 2.5: Altitude from a vertex of an isometrically realized configuration, which was chosen randomly as distances between 5 points of $\mathbb{R}^4$



Remark 11. From the realizability conditions we see, that what determines realizability is the signature of a certain matrix or equivalently the sign of principal minors. Hence the formula for the derivative of a determinant is instrumental in determining whether a critical curvature is a right or left endpoint.

Consider $\mathbf{C}_\kappa(X)$ (or $\mathcal{C}_\kappa(X)$) as a curve of matrices parameterized by $\kappa \in \mathbb{R}$, then:

$$\frac{d}{d\kappa}\det(\mathbf{C}_\kappa(X)) = \operatorname{trace}(\operatorname{cof}(\mathbf{C}_\kappa(X))\frac{d}{d\kappa}\mathbf{C}_\kappa(X)) \tag{2.57}$$

A formula which by Proposition 8 has a very geometric interpretation. The signs of the elements in $\operatorname{cof}(\mathbf{C}_\kappa(X))$ are determined by whether dihedral angles are acute or obtuse.

Relation to Volume

It is an interesting question how the volume of an isometrically realized simplex behaves as a function of curvature. If it was possible to show e.g. that $\operatorname{vol}(\Delta(X))(\kappa)$ was "concave" as a function of κ, with an appropriate notion of concavity when $\inf \mathcal{K}_X = -\infty$, then it would follow that $\mathcal{K}_X$ was connected. And then it would be natural to define the "curvature" of X as the κ where the volume was maximal. However it is not so easy to study the volume as a function of curvature. One could try as in Example 7, and perhaps an argument could be carried out in general?

If it is not easy to determine the behavior of the volume it turns out that the *complementary dual volume*, the measure of the oriented hypersurfaces intersecting $\Delta(X)$, turns out to behave simply:

Define an *expansion* of a finite subset $X \subset \mathbb{M}(n,\kappa)$ as a smooth variation $t \mapsto X_t = \{p_1(t), \ldots, p_m(t)\}$ such that $X_0 = X$ and all the distances $d(p_i(t), p_j(t))$ are strictly increasing.

For the terminology used in the following lemma see Remark 8, Example 6 and Definition 15. See also [31] and [20].

Lemma 8. *Let $X \subset \mathbb{M}(n,\kappa)$ be a vertex set spanning a simplex and let $t \mapsto X_t \subset \mathbb{M}(n,\kappa)$ be an expansion of X, then the complementary dual volume of the convex hull $\mu(\Delta(X_t)^*)$ is strictly increasing.*

Proof. For $\kappa > 0$ and a spherical simplex, $\Delta(X_t)$, the exterior dihedral angles of the polar dual $\Delta(X_t^*)$ is equal to the distances between points in X_t, which are strictly increasing. Then from the the Schläfli formula (Example 6), the volume of the polar dual is strictly decreasing. But this implies that the complementary dual volume, the measure of the set of oriented hypersurfaces intersecting $\Delta(X)$, is strictly increasing.

For $\kappa < 0$ this follows from an identical argument using the Schläfli formula established for the volume of the complementary dual in [31], Lemma 2.1.

For $\kappa = 0$ the result follows by a limit argument or by establishing a similar formula for the complementary dual volume. We shall not need this however. □

Remark 12. Note that the statement above is not valid if "complementary dual volume" is replaced by "volume"! We can have an expansion, that decreases volume.

When a finite metric space X is embedded isometrically in $\mathbb{M}(n, \kappa)$, the set of angels between directions seen from a point $p \in X$ are strictly increasing as a function of curvature, by Toponogov's Theorem; this is also seen easily directly by differentiating the cosine relation. Hence the "angle space" $\Theta \subset \mathbb{S}(n, 1)$ is expanding. Using this and the previous lemma, it is possible to show the following fact, which does seem to fit with "geometric intuition"; the proof will be omitted here though...

Proposition 11. *Suppose that $X \overset{isom}{\hookrightarrow} \mathbb{M}(n, \kappa)$ is a convexly dependent set or if $\kappa > 0$ a set such that the convex hull of X is the entire sphere $\mathbb{S}(n, \kappa)$, then κ is a right endpoint.*

Final Question: Intuition suggests that $\mathcal{K}_X$ should always be connected, with X realized as special critical configurations in the endpoints of $\mathcal{K}_X$. This is true generically, but is the question posed really so "natural" that it must always be true?

Chapter 3

Leaf Spaces

3.1 Leaf Spaces are Hyperbolic

In this chapter we shall apply some of the theory of $\mathbf{C}_\kappa$-matrices to an interesting class of metric spaces, the so called *leaf spaces*. A leaf space appears as the set of endpoints, i.e. degree 1 vertices, of a weighted tree. In particular we shall examine the question: *which metric spaces are realizable in* $\mathbb{H}(m,\kappa)$ *in the limit* $\kappa \to -\infty$. In order to economize let us introduce the terminology:

Definition 16. A metric space X will be said to satisfy condition $\mathcal{H}$ if there exists an integer m and a $\kappa_0 < 0$, such that $X \overset{isom}{\hookrightarrow} \mathbb{H}(m,\kappa)$ for all $\kappa < \kappa_0$.

With the notation of section 2.7, this is the same as $\mathcal{K}_X \neq \emptyset$ and $\inf \mathcal{K}_X = -\infty$.

Refer to 2.6 or the book [7] for conventions regarding graphs. A *finite metric space* X which is isometric to a subset of a weighted tree, will be called *tree realizable*. It is well known, and easy to prove, that if X is tree realizable, there is a unique *minimal* weighted tree $T = (V, E, w)$, such that $X \overset{isom}{\hookrightarrow} T$. We will always assume that the realizations in discussion are minimal and will often identify X with the realization in T. Hence $\deg(v)$, for $v \in X$, will mean the degree of the corresponding vertex in the realization. Points corresponding to vertices v with $\deg(v) > 1$ will be called *branch points,* while a point corresponding to a vertex of degree 1 shall be called a *leaf*.

Definition 17. A leaf space is a finite metric space that can be realized as the set of degree 1 vertices of a weighted tree $T = (V, E, w)$.

Example 10. Let $\mathrm{Star}(n,l)$ denote the *regular star graph* with radius l and n leaves. It consists of one vertex of degree n and n vertices of degree 1, the *leaves*. The n edges connecting the center to the leaves are all assumed to have length l, hence $\mathrm{diam}(\mathrm{Star}(n,l)) = 2l$. The leaf space of $\mathrm{Star}(n,l)$ is clearly realizable as a regular simplex in $\mathbb{H}(n-1,\kappa)$ for all $\kappa < 0$.

For reasons which should become clear later (see e.g. Corollary 4 below) it will be interesting to consider yet another matrix besides $\mathbf{C}_\kappa(X)$. For a finite metric space X with distance matrix $\mathbf{D} = [d_{ij}]$, and for $t \in \mathbb{R}$, we will use the notation:

$$\mathcal{E}_t(X) := [\exp(td_{ij})]$$

For $t = 1$, we will just write $\mathcal{E}(X)$.

Remark 13. If a metric space is of *negative type*, see chapter 4, then $\mathcal{E}_{-t}(X)$ is positive semidefinite for $t \geq 0$, see [7]. It is known that subsets of $\mathbb{M}(m, \kappa)$ are of negative type, chapter 4, hence $\mathcal{E}_{-t}(X)$ will be positive semidefinite for such spaces, e.g. if X satisfies condition $\mathcal{H}$.

Proposition 12. *If* $X \overset{isom}{\hookrightarrow} \mathbb{H}(m, \kappa)$ *then* $\mathcal{E}_t(X)$ *has exactly one positive eigenvalue for* $t = \sqrt{-\kappa}$.

Proof. For $\kappa < 0$ we have $\mathbf{C}_\kappa(X) = \frac{1}{2}(\mathcal{E}_t(X) + \mathcal{E}_{-t}(X))$, where $t = \sqrt{-\kappa}$. Since $X \overset{isom}{\hookrightarrow} \mathbb{H}(m, \kappa)$, $\mathbf{C}_\kappa(X)$ has exactly one positive eigenvalue. But the matrix $\mathcal{E}_{-t}(X)$ is positive semidefinite, so $\mathcal{E}_t(X)$ can have at most (and hence exactly) one positive eigenvalue. $\square$

The result below follows from Corollary 2 and 3, and is the main sum-up of the results in this chapter.

Theorem 4 (Main Theorem). *A finite metric space satisfies condition $\mathcal{H}$ if and only if it is a leaf space or a subset of the line.*

Definition 18 (The 4-point condition/0-hyperbolicity). A metric space X is said to be 0-hyperbolic, or to satisfy the 4-point condition, iff all 4-point subsets $\{p_{i_1}, p_{i_2}, p_{i_3}, p_{i_4}\} \subseteq X$ satisfy the following: Among the three sums

$$s_1 = d_{i_1 i_2} + d_{i_3 i_4}, s_2 = d_{i_1 i_3} + d_{i_2 i_4}, s_3 = d_{i_1 i_4} + d_{i_2 i_3}, \tag{3.1}$$

two are equal and not smaller than the third one.

We have, cf. [12]:

Theorem 5. *A finite metric space is tree realizable iff it is 0-hyperbolic.*

Remark 14. In Gromov's theory of δ-hyperbolic spaces (see [12]), 0-hyperbolic spaces appear as *asymptotic subcones*. That a metric space is an asymptotic subcone of hyperbolic space of curvature -1 means that it is embeddable at "infinity", and this is a weaker condition than condition $\mathcal{H}$, where we require embeddability “before infinity”. The least δ, such that a space X is δ-hyperbolic, can be used to give bounds on the left endpoint of $\mathcal{K}_X$, since we have that the hyperbolic spaces $\mathbb{H}(m, \kappa)$ are δ_κ-hyperbolic, with $\delta_\kappa \to 0$ for $\kappa \to -\infty$.

Hence it already follows from this theory , that a space satisfying condition $\mathcal{H}$ must be 0-hyperbolic, and then must be either a leaf space or a subset of the line (there can be no "branching geodesics") . However we shall treat the problem in a self contained way, using the Gram matrix machinery, without reference to δ-hyperbolic spaces.

This particular result, the "only if" part, appears as an easy consequence of the matrix theory though:

Proposition 13. *A metric space on* 4 *points that satisfies condition* $\mathcal{H}$ *is a leaf space or a subset of the line.*

Proof. Simply expanding the determinant of $\mathcal{E}_t(X)$, where $X = \{p_1, p_2, p_3, p_4\}$, and collecting possible candidates for a leading order exponent, reveals:

$$\begin{aligned}\det(\mathcal{E}_t(X)) = &-2\exp(t(d_{12}+d_{23}+d_{34}+d_{41})) \\ &- 2\exp(t(d_{12}+d_{24}+d_{43}+d_{41}) - 2\exp(t(d_{13}+d_{32}+d_{24}+d_{41}) \\ &+ \exp(2t(d_{12}+d_{34})) + \exp(2t(d_{13}+d_{24})) + \exp(2t(d_{14}+d_{23})) \\ &+ \text{ lower order terms}\end{aligned} \tag{3.2}$$

Here the first three terms correspond to the six 4-cycles in Σ_4; these have negative sign. The last three terms correspond to elements composed of two 2-cycles, which gives a positive sign. It is easily seen that if one of the three sums s_1, s_2, s_3 as defined in Theorem 18, is strictly larger than the two others, then the leading order exponent in (3.2) occurs in one of the last 3 terms. Hence the sign of the determinant would be positive for t large, and X could not be embeddable in $\mathbb{H}(m, \kappa)$, where $\kappa = -t^2$, by Proposition 12.

Hence s_1, s_2, s_3 does not have a strict maximum, so that X is tree realizable by Theorem 18. Since $\mathbb{H}(m, \kappa)$ does not have "branching geodesics", it is clear that X must either be a leaf space or a subset of the line (all branch points have degree 2). ☐

If X satisfies condition $\mathcal{H}$ then the same is true for all 4-point subsets, and hence X satisfies the 4-point condition, so as a corollary to the proposition we get (with the same argument, that $\mathbb{H}(m, \kappa)$ does not have "branching geodesics").

Corollary 2. *Let X be a finite metric space. If X satisfies condition $\mathcal{H}$ then X is a leaf space or a subset of the line.*

Let us turn our attention to the opposite direction, are all leaf spaces embeddable in $\mathbb{H}(m, \kappa)$ when the curvature is negative enough? In fact we will show a little more:

Theorem 6. *Let $X = \{v_1, \dots, v_n\}$ be a tree realizable metric space with b branch points. Then the eigenvalues $\{\lambda_1, \dots, \lambda_n\}$ of $\mathbf{C}_\kappa(X)$ converge in $\mathbb{R} \cup \{\pm\infty\}$ for $\kappa \to -\infty$ and can be ordered such that*

$$\lim_{\kappa \to -\infty} \lambda_n = +\infty \textit{ and } \lim_{\kappa \to -\infty} \lambda_i = -\infty \textit{ for } i = b+1..n-1 \tag{3.3}$$

$$\lim_{\kappa \to -\infty} \lambda_i = \frac{\deg(v_i) - 2}{2(\deg(v_i) - 1)} \textit{ for } i = 1 \dots b. \tag{3.4}$$

We see that if $T = (V, E, w)$ is a weighted tree, it is clearly possible to construct a procedure using Theorem 6 to recover the combinatorial structure of T from the limits of eigenvalues of the $\mathbf{C}_\kappa$-matrix of T and certain subspaces.

Proposition 14. *Let $T = (V, E, w)$ be a weighted tree. From the limits, as $\kappa \to -\infty$, of eigenvalues of $\mathbf{C}_\kappa(T)$ and its principal submatrices the combinatorial structure of T can be recovered.*

Using Proposition 15 below, also the weight function can be recovered.

Since a leaf space has no branch points, the $\mathbf{C}_\kappa$-matrix will for large negative κ have exactly 1 positive eigenvalue, so by Theorem 1 we get:

Corollary 3. *All leaf spaces satisfy condition $\mathcal{H}$.*

This concludes the proof of Theorem 4 modulo the proof of Theorem 6, which is given below.

Proof of Theorem 6

We shall work first with the $\mathcal{E}$-matrix and deal later with the $\mathbf{C}_\kappa$-matrix. Clearly there is a unique expansion

$$\det[\exp(d_{ij})] = \sum_{k \in I} c_k \exp(\omega_k), \tag{3.5}$$

such that $\omega_k = \omega_l$ iff $k = l$, where I is a finite index set. The c_k's will be integers determined by the combinatorics and each ω_k a linear combination of the edge lengths in the tree representing X. ω_{max} will be used to denote the leading order exponent in the expansion $\omega_{max} := \max_{k \in I} \omega_k$, and c_{max} will be the corresponding coefficient.

Proposition 15. *Let X be a tree realizable metric space and $T = (V, E, w)$ the weighted tree that represents X. Then*

$$\omega_{max}(X) = 2L(X) \quad \text{and} \quad c_{max}(X) = (-1)^{|X|+1} \prod_{v \in V \setminus X} (\deg(v) - 1), \tag{3.6}$$

where $L(X) := \sum_{e \in E} w(e)$ is the total weight. *And if X is a full tree, i.e. $X = V$, then*

$$\det(\mathcal{E}(X)) = \prod_{e \in E} (1 - \exp(2w(e))) \tag{3.7}$$

Proof. We will describe two operations from which any tree realizable metric space can be constructed. Let $T = (V, E, w)$ be a weighted tree and assume that all subsets $X \subseteq V$ satisfies Proposition 15.

Operation A If $v \in X \subseteq V$ is a leaf, consider the new tree $\tilde{T}$, where $k \geq 1$ leaves $\{l_1, \ldots, l_k\}$ have been attached to v by edges of weight w_i, $1 \leq i \leq k$. Let $\tilde{X}$ consist of $X \cup \{l_1, \ldots, l_k\}$. Clearly $d(l_i, x) = d(v, x) + w_i$ for any $x \in \tilde{X} \setminus \{l_i\}$. Order the points of $\tilde{X}$ such that l_i is the i'th point and v is point number $k + 1$ and consider the matrix $\mathcal{E}(\tilde{X})$.

Now multiply row $k+1$ by $\exp(w_i)$ and subtract the result from row i for $i = 1 \dots k$. This will produce a matrix of the form:

$$\begin{pmatrix} \Lambda & O \\ A & \mathcal{E}(X) \end{pmatrix}$$

Where Λ is a $k \times k$ diagonal matrix with diagonal entries $\lambda_{i,i} = 1 - \exp(2w_i)$, and O is a $k \times |X|$ matrix of zeros. Hence

$$\det(\mathcal{E}(\tilde{X})) = \prod_{i=1}^{k} (1 - \exp(2w_i)) \det \mathcal{E}(X) \tag{3.8}$$

We see that $\omega_{max}(\tilde{X}) = 2\sum_{i=1}^{k} w_i + \omega_{max}(X)$ and $c_{max}(\tilde{X}) = (-1)^k c_{max}(X)$. If X satisfied (3.6) above, this will then also be true for $\tilde{X}$. Hence this operation of *adding branches to a leaf* preserves (3.6). It is clear that a full tree can be built using only operation A, so (3.7) follows by induction from (3.8).

Operation B Now consider again a leaf $v \in X \subseteq V$ and attach $k \geq 2$ new leaves, but let $\tilde{X}$ consist of $(X \setminus \{v\}) \cup \{l_1, \dots, l_k\}$, so that the branch point v is not included in $\tilde{X}$. Order the points so that l_i is the i'th point of $\tilde{X}$. Consider the two first leaves l_1, l_2, and let x be any other point of $\tilde{X}$, then $d(l_1, x) = d(l_2, x) + w_1 - w_2$. Hence multiplying row 2 of $\mathcal{E}(\tilde{X})$ by $\exp(w_1 - w_2)$ and subtracting the result from row 1 will produce zeros in the first row beyond the second column. Do the same thing for the first and second column. The following happens to the principal submatrix involving l_1 and l_2:

$$\begin{pmatrix} 1 & e^{w_1+w_2} \\ e^{w_1+w_2} & 1 \end{pmatrix} \sim \begin{pmatrix} 1 - e^{2w_1} & e^{w_1+w_2} - e^{w_1-w_2} \\ e^{w_1+w_2} & 1 \end{pmatrix} \sim$$
$$\begin{pmatrix} 1 - 2e^{2w_1} + e^{2(w_1-w_2)} & e^{w_1+w_2} - e^{w_1-w_2} \\ e^{w_1+w_2} - e^{w_1-w_2} & 1 \end{pmatrix}$$

Expanding the whole determinant of

$$\begin{pmatrix} 1 - 2e^{2w_1} + e^{2(w_1-w_2)} & e^{w_1+w_2} - e^{w_1-w_2} & 0 & \cdots \\ e^{w_1+w_2} - e^{w_1-w_2} & 1 & e^{d_{23}} & \cdots \\ 0 & e^{d_{23}} & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

we get:

$$\det \mathcal{E}(\tilde{X}) = (1 - 2e^{2w_1} + e^{2(w_1-w_2)}) \det \mathcal{E}(\tilde{X}_1) - (e^{w_1+w_2} - e^{w_1-w_2})^2 \det \mathcal{E}(\tilde{X}_{12}),$$

where $\tilde{X}_1$ denotes the subspace of $\tilde{X}$ with the point l_1 deleted, and $\tilde{X}_{12}$ has l_1, l_2 deleted. Collecting maximal terms we get:

$$\det \mathcal{E}(\tilde{X}) = -2c_{max}(\tilde{X}_1)e^{2w_1+\omega_{max}(\tilde{X}_1)} - c_{max}(\tilde{X}_{12})e^{2(w_1+w_2)+\omega_{max}(\tilde{X}_{12})} + \text{lower order terms} \tag{3.9}$$

For $k = 2$, $\tilde{X}_1$ is combinatorially the same as X except that the length of the edge that contains l_2, which corresponds combinatoricly to $v \in X$, has been increased by w_2. And $\tilde{X}_{12}$ is the subspace of X in which the leaf v has been removed, hence by induction assumption $\omega_{max}(\tilde{X}_{12}) = 2L(X) - 2w(e_v)$, where v_e is the edge of T that contains the leaf v, and also $\omega_{max}(\tilde{X}_1) = 2L(X)+2w_2$. Hence we see that $\omega_{max}(\tilde{X}) = 2L(X)+2w_2+2w_1 = 2L(\tilde{X})$ and $c_{max}(\tilde{X}) = -2c_{max}(\tilde{X}_1) = -2c_{max}(X)$. The last equality because $\tilde{X}_1$ and X are combinatorially equivalent. Now for $k > 2$,by induction in k, the two exponents in (3.9) are both equal to $2L(\tilde{X})$, and $c_{max}(\tilde{X})$ becomes $-2c_{max}(\tilde{X}_1) - c_{max}(\tilde{X}_{12})$ which (by induction) is easily seen to be $k(-1)^{k-1}c_{max}(X)$.

Since both operation A and operation B preserves (3.6), and any tree realizable metric space X can be built using these two operations the result follows by induction. □

Remark 15. This maximal "surviving" frequency in the expansion of $\det(\mathcal{E}(X))$, $\omega_{max}(X)$, does seem to be an interesting number connected to a metric space. $\frac{1}{n}\omega_{max}(X)$ is some kind of combinatorial mean distance, a measure of the size of X.

From simple combinatorial considerations, using the definition of a determinant, it can be seen directly, that each exponent in

$$\det[\exp(d_{ij})] = \sum_{k\in I} c_k \exp(\omega_k),$$

that involves the distance to a leaf l_i, must contain the weight w_i of the edge containing l_i with a factor of two. That is $\omega = 2w_i +$ terms without w_i, for any exponent involving w_i. This was not used in the proof above, but shall be utilized in:

Corollary 4. *The $\mathcal{E}(X)$-matrix of a tree realizable metric space is regular and has 1 positive eigenvalue and $|X| - 1$ negative eigenvalues.*

Proof. From Proposition 15 it follows that if V is the vertex set of a tree $T = (V, E, w)$, then $\mathcal{E}(V)$ is regular and the determinant has sign $(-1)^{|V|+1}$, since $|E| = |V| - 1$.

There is a sequence of subtrees with vertex sets V_i such that $|V_i| = i$, $i = 1 \ldots |V|$ (e.g. by "peeling off leaves"). Hence $\mathcal{E}(V)$ has an alternating sequence of increasing principal minors. The result for $\mathcal{E}(V)$ then follows from linear algebra, see [9].

But then for any subspace $X \subseteq V$, since the $\mathcal{E}(X)$-matrix is a principal minor it can have at most one positive eigenvalue. Hence it must have exactly one positive eigenvalue, and the determinant will have sign $(-1)^{|X|+1}$ if nonvanishing. So if $\det(\mathcal{E}(X)) = 0$ then $\frac{d}{dw_i}\det(\mathcal{E}(X)) = 0$, where w_i is the weight of some edge in the tree. If w_i is the weight of an edge that contains a leaf $l_i \in X$, then

$$\frac{d}{dw_i}\det(\mathcal{E}(X)) = \frac{d}{dw_i}\sum_{k\in I} c_k \exp(\omega_k) = -2w_i \det(\mathcal{E}(X_i)),$$

where X_i is the subspace with l_i deleted. This is because all the terms that doesn't include w_i gives the expansion of $\det \mathcal{E}(X_i)$, hence the terms which include w_i is equal to $\det(\mathcal{E}(X)) - \det(\mathcal{E}(X_i)) = -\det(\mathcal{E}(X_i))$. Now the result follows by induction, assuming $\mathcal{E}(X_i)$ is regular. □

Lemma 9. *Let* $p : \mathbb{R}_+ \to P_n(\mathbb{R}),\ t \mapsto p_t(\lambda) = \sum_{i=0}^n a_i(t)\lambda^i$*, be a curve of polynomials of degree* n*. Assume that all the fractions* $\frac{a_i(t)}{a_0(t)}$ *converge for* $t \to \infty$*, and let* j *be the maximal index such that:*

$$\lim_{t\to\infty} \frac{a_i(t)}{a_0(t)} = 0 \text{ for } i > j$$

Then p_t *will have* $n-j$ *roots that converge to* ∞ *in numerical value, and* j *bounded roots which will converge to the roots of* $q(\lambda) = \sum_{i=0}^j b_i\lambda^i$*, where* $b_i = \lim_{t\to\infty} \frac{a_i(t)}{a_0(t)}$*,* $i = 0 \dots j$

Proof. This is just a special case of a more general principle for homotopies, or sequences, of holomorphic functions, which can be stated as: during a homotopy of holomorphic functions, the zeros move continuously in $\mathbb{C}$, and no zeros disappears except to ∞.

Alternatively, consider the polynomial: $\tilde{p}_t(\lambda) := \frac{\lambda^n}{a_0(t)} p_t(\frac{1}{\lambda})$, and use that (assuming $a_0(t) \neq 0$) there is a $1-1$ correspondence between the roots of p_t and $\tilde{p}_t : \lambda_i \mapsto \frac{1}{\tilde{\lambda}_i}$. □

Lemma 10. *Let* $X = \{v_1, \dots, v_n\}$ *be a tree realizable metric space with b branch points. Then the eigenvalues* $\{\lambda_1, \dots, \lambda_n\}$ *of* $\mathcal{E}_t(X)$ *converge in* $\mathbb{R} \cup \{\pm\infty\}$ *for* $t \to \infty$ *and can be ordered such that*

$$\lim_{t\to\infty} \lambda_n = +\infty \text{ and } \lim_{t\to\infty} \lambda_i = -\infty \text{ for } i = b+1..n-1 \tag{3.10}$$

$$\lim_{t\to\infty} \lambda_i = \frac{-1}{\deg(v_i)-1} \text{ for } i = 1 \dots b. \tag{3.11}$$

Proof. We have $\det(\mathcal{E}_t(X)) = c_{max}(X)\exp(\omega_{max}(X)t) + o(\exp(\omega_{max}t))$, and $\omega_{max}(X) = 2L(X)$, by Proposition 15. Let $\{v_1, \dots, v_b\}$ be the branch points of X.

It is clear that for $j \leq b$ and $Y = X \setminus \{v_1, \dots, v_j\}$, we have $L(Y) = L(X)$. So $\omega_{max}(Y) = \omega_{max}(X)$ and $c_{max}(Y) = c_{max}(X)(-1)^j \prod_{k=1}^j(\deg(v_k)-1)$. On the other hand, removing a leaf $l \in X$ will decrease $L(X \setminus \{l\})$ by the weight of the edge that contains l. Hence any principal minor of $\mathcal{E}_t(X)$ corresponding to having removed a leaf will be $o(\det \mathcal{E}_t(X))$, whereas for any minor corresponding to having removed branch points $\{v_1, \dots, v_j\}$, we have

$$\lim_{t\to\infty} \frac{\det \mathcal{E}_t(Y)}{\det \mathcal{E}_t(X)} = \frac{c_{max}(Y)}{c_{max}(X)} = (-1)^j \prod_{k=1}^j (\deg(v_k)-1)$$

If now $a_i(t)$ is the coefficient of λ^i in the characteristic polynomial of $\mathcal{E}_t(X)$, then since $a_i(t)$ is (up to a sign) the sum of all principal minors of size $n-i$, for $i > b$ each minor must have removed a leaf and hence have strictly less leading exponent. So we get $\lim_{t\to\infty} \frac{a_i(t)}{a_0(t)} = 0$ for $i > b$, where b is the number of branch points of X. And for $i \leq b$ we get $\lim_{t\to\infty} \frac{a_i(t)}{a_0(t)} = b_i \neq 0$.

Lets try to determine the coefficients in this "limiting" polynomial $q(\lambda) = \sum_{i=0}^{b} b_i \lambda^i$. Clearly $b_0 = 1$. For $i > 0$, it is easily seen that

$$b_i = \sum_{|J|=i} (-1)^i \prod_{k\in J} (\deg(v_k) - 1), \tag{3.12}$$

a sum over all $J \subseteq \{1, \ldots, b\}$, with $|J| = i$. But we see that the coefficients in

$$\prod_{k=1}^{b} (1 - [\deg(v_k) - 1]\lambda) \tag{3.13}$$

are exactly given by (3.12). Hence the roots of $q(\lambda)$ are $\lambda_i = \frac{-1}{\deg(v_i)-1}$ $i = 1 \ldots b$. The result now follows by Lemma 9.

□

Now we shall get back to the $\mathbf{C}_\kappa(X)$ matrix. For $\kappa < 0$ we have

$$\mathbf{C}_\kappa(X) = \frac{1}{2}\big(\mathcal{E}_t(X) + \mathcal{E}_{-t}(X)\big), \tag{3.14}$$

where $t = \sqrt{-\kappa}$. Since the second term $\mathcal{E}_{-t}(X)$ converges to the identity matrix for $t \to \infty$, the result follows directly from Lemma 10, taking the factor $\frac{1}{2}$ into account.

This finishes the proof of Theorem 6. □

3.2 The Limiting Geometry

It has been shown that any leaf space X on n points can be isometrically embedded as a simplex in $\mathbb{H}(n-1, \kappa)$, when the curvature κ is negative enough. Intuition tells us, that the simplex should get more "skinny", resembling the tree that represents X more as $|\kappa|$ increases. A few descriptive results on the limiting geometry, will be presented in this section.

As before we let h_i be the altitude from p_i onto the hypersurface spanned by $X - \{p_i\}$. We have:

Proposition 16. *Let $X = \{p_1, \ldots, p_n\}$ be a leaf space. Then $\lim_{\kappa\to-\infty} h_i = w_i$, where w_i is the weight of the edge in T that contains p_i.*

Proof. As for $\det(\mathcal{E}_t(X))$, cf. equation (3.5), we have an expansion

$$\det(\mathbf{C}_\kappa(X)) = \sum_{k\in I} c_k \exp(\omega_k t), \tag{3.15}$$

where $t = \sqrt{-\kappa}$. Here the leading order exponent must be as for $\det(\mathcal{E}_t(X))$, $\omega_{max} = 2L(X)$. This can be seen by a non-combinatorial argument:

We have $2\mathbf{C}_\kappa(X) - \mathcal{E}_t(X) = \mathcal{E}_{-t}(X)$, multiplying by $\mathcal{E}_t(X)^{-1}$ and rearranging we get

$$2\mathbf{C}_\kappa(X)\mathcal{E}_t(X)^{-1} = \mathcal{E}_{-t}(X)\mathcal{E}_t(X)^{-1} + \mathbf{I} \tag{3.16}$$

Now, the right hand side will converge to $\mathbf{I}$ for $t = \sqrt{-\kappa} \to \infty$. This is true because $\mathcal{E}_{-t}(X) \to \mathbf{I}$ and $\mathcal{E}_t(X)^{-1} \to \mathbf{0}$ for $t \to \infty$, since X doesn't contain branch points (cf. Theorem 6). Hence the claim follows by taking determinants.

We have

$$\log(|\det(\mathbf{C}_\kappa(X))|) = \\ \log|\sum_{k\in I} c_k \exp(\omega_k t)| = \omega_{max} t + \log|c_{max} + \sum_{\omega_k \neq \omega_{max}} (c_k \exp((\omega_k - \omega_{max})t)| \quad (3.17)$$

Hence $\frac{\log(|\det(\mathbf{C}_\kappa(X))|)}{t} \to \omega_{max} = 2L(X)$ for $t = \sqrt{-\kappa} \to \infty$. Using Theorem 2 we get, assuming for the sake of notation that $i = n$:

$$\log(|\det(\mathbf{C}_\kappa(X))|) = \sum_{j=2}^{n} 2(h_{<j} t + \log(\frac{1 - exp(-2th_{<j})}{2}) \quad (3.18)$$

Dividing by t and taking the limit $t \to \infty$ we get: $2\sum_{j=2}^{n} h_{<j} = 2L(X)$. The result follows by induction using $L(X - \{p_n\}) = L(X) - w_n$. □

Let now $\tilde{\theta}_{ij}$ denote the *interior* dihedral angle at the co-dimension 2 face $\Delta(X_{ij})$. Let $T = (V, E, w)$ be the weighted tree that represents X, and for $p \in X$ let $v(p) \in V$ be the branch point of T such that $v(p)$ is adjacent to p. Then we have:

Proposition 17. *Let $X = \{p_1, \ldots, p_n\}$ be a leaf space. Then for $i \neq j$:*

$$\lim_{\kappa \to -\infty} \tilde{\theta}_{ij} = \begin{cases} \mathrm{Arccos}(\frac{1}{(\deg(v)-2)}) & \text{if } v(p_i) = v(p_j) \\ \frac{\pi}{2} & \text{if } v(p_i) \neq v(p_j) \end{cases} \quad (3.19)$$

Proof. By (3.16) we determine that the leading order exponent ω_{max} and the corresponding coefficient c_{max} in the expansions of $\det(\mathbf{C}_\kappa(X))$ and $\det(\mathcal{E}_t(X))$ (3.15) and (3.5) satisfies:

$$c_{max,\mathbf{C}_\kappa}(X) = 2^{-n} c_{max,\mathcal{E}}(X), \quad \omega_{max,\mathbf{C}_\kappa}(X) = \omega_{max,\mathcal{E}}(X) = 2L(X) \quad (3.20)$$

Also by the proof of Proposition 8:

$$\frac{\det(\mathbf{C}_\kappa(X_{ij}))\det(\mathbf{C}_\kappa(X))}{\det(\mathbf{C}_\kappa(X_i))\det(\mathbf{C}_\kappa(X_j))} = \sin(\tilde{\theta}_{ij})^2 \quad (3.21)$$

Assuming at first that $v(p_i) = v(p_j) := v$, then the total weights satisfy $L(X_i) = L(X) - w_i$, $L(X_j) = L(X) - w_j$ and $L(X_{ij}) = L(X) - w_i - w_j$, unless $\deg(v) = 3$ in which case $L(X_{ij}) < L(X) - w_i - w_j$, with notation as earlier. Inserting in (3.21), we see that

$$\sin(\tilde{\theta}_{ij})^2 \to \frac{c_{max}(X_{ij})c_{max}(X)}{c_{max}(X_i)c_{max}(X_j)}, \quad (3.22)$$

if $\deg(v) > 3$, and $\sin(\tilde{\theta}_{ij})^2 \to 0$ if $\deg(v) = 3$. Assuming $\deg(v) > 3$ we get by Proposition 15: $\frac{c_{max}(X)}{c_{max}(X_i)} = -\frac{\deg(v)-1}{\deg(v)-2}$ and $\frac{c_{max}(X_{ij})}{c_{max}(X_j)} = -\frac{\deg(v)-3}{\deg(v)-2}$. It is left to show, that the interior dihedral angles are acute. For this we refer to Lemma 11 below.

The case $v(p_i) \neq v(p_j)$ is similar, but here the quotient in (3.22) is seen to be 1. □

The result in the case where $\lim \tilde{\theta}_{ij} = \operatorname{Arccos}(\frac{1}{(\deg(v)-2})$ seems a bit surprising, since $\lim h_i = \lim h_{ij} = w_i$ (with notation as in the proof of Proposition 8). But the finer details of the convergence are needed, and these could be found from (3.17) and (3.18).

Lemma 11. *Let X be a leaf space. There is a $\kappa_0 < 0$ such that $\kappa < \kappa_0$ implies:* $X \overset{isom}{\hookrightarrow} \mathbb{H}(|X| - 1, \kappa)$ *and all interior dihedral angles $\tilde{\theta}_{ij}$ corresponding to leaves with $v(p_i) = v(p_j)$ are acute.*

Proof. Again we shall because of the easier algebra work with $\mathcal{E}_t(X)$. Let $p_i, p_j \in X$ have $v(p_i) = v(p_j)$. Then for every $q \in X_{ij} = X \setminus \{p_i, p_j\}$:

$$d(q, p_i) = d(q, p_j) - w_j + w_i \tag{3.23}$$

Let $[c_{kl}]$ be the components of $\operatorname{cof}(\mathcal{E}_t(X))$. $c_{ij} = (-1)^{i+j}|\mathcal{E}_t(X)^i_j|$ is the signed minor obtained by deleting column i and row j. Expanding the minor after column j of $\mathcal{E}_t(X)$, the obtained minors can be interpreted as minors of the principal submatrix $\mathcal{E}_t(X_j) = \mathcal{E}_t(X)^j_j$, where $X_j := X \setminus \{p_j\}$. Assume that $i < j$, then we get since column j of $\mathcal{E}_t(X)$ is column $j-1$ of $\mathcal{E}_t(X_j)^i_j$:

$$c_{ij} = (-1)^{i+j}\Bigg(\sum_{k=1}^{j-1}(-1)^{j-1+k}\exp(td_{kj})|\mathcal{E}_t(X_j)^i_k| + \\ \sum_{k=j}^{|X|-1}(-1)^{j-1+k}\exp(td_{k+1,j})|\mathcal{E}_t(X_j)^i_k|\Bigg)$$

Multiplying by $\exp(t(w_i - w_j))$ and using (3.23), it is seen that we almost get the expansion of $\det(\mathcal{E}_t(X_j))$, except for a sign and the coefficient in the term with $k = i$, i.e. the coefficient of $|\mathcal{E}_t(X_j)^i_i| = \det(\mathcal{E}_t(X_{ij}))$:

$$c_{ij}\exp(t(w_i - w_j)) = -\det(\mathcal{E}_t(X_i)) - (\exp(2w_i) - 1)\det(\mathcal{E}_t(X_{ij})) \tag{3.24}$$

Using Proposition 15, we see that both terms on the right hand side have the same leading order exponent, but that the first term has largest coefficient and is dominant as $t \to \infty$. Hence the sign of c_{ij} will be as for $\det(\mathcal{E}_t(X))$ for t large.

Now using $2\mathbf{C}_\kappa(X) = \mathcal{E}_t(X)(\mathbf{I} + \mathcal{E}_t(X)^{-1}\mathcal{E}_{-t}(X))$, the result follows for $\mathbf{C}_\kappa(X)$ by taking cofactors, since $\mathcal{E}_t(X)^{-1}\mathcal{E}_{-t}(X) \to \mathbf{0}$ for $t = \sqrt{|\kappa|} \to \infty$. It follows from (2.26) that the exterior dihedral angle θ_{ij} will have negative cosine, and hence the interior dihedral angle will be acute. □

Claim: In fact with a little more combinatorial insight[1] it is possible to show, that for a leaf space X, all cofactors will have the same sign as $\det(\mathbf{C}_\kappa(X))$ in the limit $\kappa \to -\infty$. And hence also the interior angles converging to $\frac{\pi}{2}$ will be acute.

[1] As promised in [18]. It is still true, but due to time pressure the details will not be given here either :-(

A regular simplex is the leaf space of a *star*, c.f. Example 10. In this case Proposition 17 can be interpreted as a result about the regular, *ideal simplex*, a simplex with all vertices on the sphere at infinity, cf. [25]:

Increasing $|\kappa|$ and considering the realization of $X \in \mathbb{H}(n,\kappa)$ as a realization of $\sqrt{|\kappa|}X$ in $\mathbb{H}(n,-1)$, which is the same thing, the of vertices of $\sqrt{|\kappa|}X$ will converge to a subset of the sphere at infinity. This regular, ideal simplex is the unique simplex of maximal volume in $\mathbb{H}(n,-1)$, cf. [11].

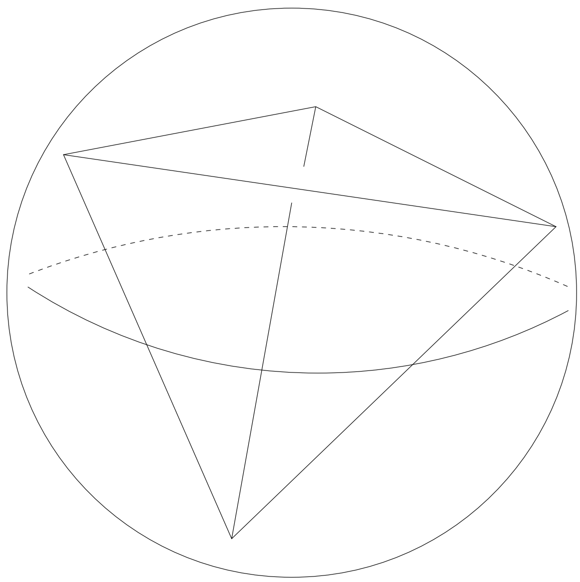
In the limit we find for the regular, ideal simplex in $\mathbb{H}(n,-1)$:

$$\cos(\tilde{\theta}_{ij}) = \frac{1}{n-1}, \text{ for } i \neq j \tag{3.25}$$

This is then interpreted as a description of the *dual ideal simplex*. Hence we have that $\mathbf{C}_\kappa(X^*) = [x_{ij}]$ with $x_{ii} = 1$ and $x_{ij} = -\frac{1}{n-1}$ (exterior dihedral angles). It is easily checked that $\mathbf{C}_\kappa(X^*)$ is regular with all codimension 1 principal minors vanishing. *X is a simplex with degenerate/lightlike codimension* 1 *faces*.

What about a leaf space which is less symmetric, will the vertices converge to the vertices of a simplex at the sphere at infinity?

Figure 3.1: An ideal simplex with vertices at the sphere at infinity.



Proposition 18. *Let X be the leaf space of a tree containing more than one branch point, then the limit of $\mathbf{C}_\kappa(X^*)$ is singular, hence the realizations of $\sqrt{|\kappa|}X$ cannot be made to converge to a simplex on the sphere at infinity for $\kappa \to -\infty$.*

Proof. Define a vector $x \in \mathbb{R}^{|X|}$ such that $x_i = 1$ whenever the corresponding leaf l_i is adjacent to an interior vertex $v(l_i)$, which again is adjacent to exactly one other interior point; and put $x_i = 0$ otherwise. It is easy to see that we do not get the zero vector when X is not the leaf space of a star: simply take any vertex in T and take a point which is furthest away with the combinatorial distance. Then this leaf and all other leaves adjacent to the same interior vertex will satisfy the requirement and get weight 1.

From Proposition 17 it is then seen that this vector is in the kernel of $\mathbf{C}_\kappa(X^*)$. $\square$

Chapter 4

Negative Type

In this part of the thesis the concept of *negative type* of metric spaces is studied, see below for the definition. It is a concept which has appeared in analysis and combinatorics in many disguises and under many different names.

In the work of Schoenberg, Blumenthal and Menger in the 1930's, [28], [2], negative type appeared in connection with a criterion for realizability of a metric space in Euclidean space, or more generally in Hilbert space, c.f. Theorem 7 below. Later it was studied by Kelly from a combinatorial viewpoint, see [16] and [17]. Also in harmonic analysis negative type has been of interest, see e.g. [8], [26] and [27]. A thorough and up to date reference is [7], which contains most of what is known about negative type, in relation to analysis, combinatorics and graph theory.

Although negative type has a long history, the concept has not been studied extensively in pure geometry and in particular in subfields such as Riemannian and Alexandrov geometry it is a non standard subject. This chapter continues the journey that was initiated in [14]; trying to get a grasp on what negative type actually means in this context.

Looking at the definition of negative type, see below, it seems surprising that any interesting spaces would actually fulfill the requirement. But it turns out that the space forms $\mathbb{M}(n, \kappa)$, defined previously, are examples of Riemannian manifolds of negative type. These spaces all have constant curvature and are simply connected (for $n \geq 2$). Several questions arise: are there examples of Riemannian manifolds of negative type, that does not have constant curvature? Does negative type have any topological implications?

Several interesting concepts appear naturally in connection with negative type. One of these is *extent* as defined in [10] and [13]. The extent of a metric space may also be seen as the *maximal mean distance* when points are distributed according to some probability measure on the space. It turns out that negative type is related to uniqueness of realizations of such quantities, which may also be viewed as *maximal energies*; this is perhaps the most geometrically significant feature of negative type.

Apart from the question of classification according to negative type in itself, perhaps the most important and rewarding feature of the subject is the new ideas and metric invariants, that seems to suggest themselves.

Several questions remain: What do Riemannian manifolds of negative type look like?

Is the constant curvature sphere the only compact example, a lone soul in this category? These questions will be addressed in the following. . .

4.1 Fundamental Properties

The first section is a sum up of some relevant material.
Convention: Whenever a double sum

$$\sum_{i,j} = \sum_i \sum_j \tag{4.1}$$

is considered, we use the convention that for $i \neq j$ both terms (i, j) and (j, i) appear. The double sum is the same as an *integral* over a finite product space.

Definition 19. Let X be a finite metric space with distance matrix $\mathbf{D} = [d_{ij}]$.

- X is of *negative type* iff

$$x^t\mathbf{D}x = \sum_{i,j=1}^{n} x_i x_j d_{ij} \leq 0 \text{ for } x \in \Pi_0(X) := \{x \in \mathbb{R}^{|X|} | \sum_{i=1}^{n} x_i = 0\}, \tag{4.2}$$

  and of *strictly negative type* if $x^t\mathbf{D}x < 0$ for $x \in \Pi_0(X) \setminus \{0\}$.

- X is *hypermetric* iff

$$x^t\mathbf{D}x = \sum_{i,j=1}^{n} x_i x_j d_{ij} \leq 0 \text{ for } x \text{ in the discrete set } \{x \in \mathbb{Z}^{|X|} | \sum_{i=1}^{n} x_i = 1\} \tag{4.3}$$

- An infinite distance space is defined to be of negative type / strictly negative type/ hypermetric iff all finite subspaces are.

- $\mathcal{NT}$, $\mathcal{SNT}$ denotes respectively the category of all spaces of negative type/strictly negative type, while $\mathcal{HYP}$ denotes the category of hypermetric spaces.

We could define negative type/hypermetricity for $\mathbb{R}_+$-distance spaces, i.e. without requiring the triangle inequality satisfied. However it is easy to see that hypermetricity implies the triangle inequality, and negative type implies that $\sqrt{d}$ is a metric, c.f. Theorem 7 below. Later we shall consider negative type of *kernels* of the form $f(d)$, where f is a modification function.

Remark 16. Note that if X is of negative type/hypermetric, the same holds for all subspaces $Y \subseteq X$.

It is an easy result that hypermetricity implies negative type, see [16].

Proposition 19. $\mathcal{HYP} \subset \mathcal{NT}$

Since hypermetricity and negative type is defined with a $\leq$-sign we have[1]:

Proposition 20. *$\mathcal{HYP}$ and $\mathcal{NT}$ are closed in the category of compact metric spaces with the Gromov-Hausdorff distance:*

Suppose that X is a compact metric space and $\{X_n\}_{n\in\mathbb{N}}$ is a sequence of compact metric spaces with $X_n \in \mathcal{HYP}$ (or $\mathcal{NT}$). Then $d_{GH}(X_n, X) \to 0 \implies X \in \mathcal{HYP}$ (or $\mathcal{NT}$).

The same thing holds for convergence of pointed noncompact spaces, so that $\mathcal{HYP}$ and $\mathcal{NT}$ are closed in the category of pointed noncompact, metric spaces.

Negative type has been of interest in analysis mainly because of of the following, c.f. [7] section 3.2. (see also page 79):

Theorem 7. *Let (X, d) be a $\mathbb{R}_+$-distance space. There is a Hilbert space $\mathcal{H}$ such that $(X, \sqrt{d}) \overset{isom}{\hookrightarrow} \mathcal{H}$ if and only if (X, d) is of negative type*

Just to show that there are lots of examples of metric spaces of negative type, we have:

Lemma 12. *If (X, d_X) and (Y, d_Y) are of negative type, then the l_1-metric $d = d_X + d_Y$ on $X \times Y$ is of negative type (the same holds for strictly negative type and hypermetricity).*

Proof. A distance matrix for d is the sum of the distance matrices for d_X and d_Y. □

Proposition 21. *Any second countable, normal topological space X has a metric of negative type, that is consistent with the topology. Any smooth manifold M^n has a metric of negative type, that is consistent with the topology and is smooth on $M \times M \setminus \{(p, p) | \, p \in M\}$*

Proof. For the first statement, realize X homeomorphically in the Tychonoff cube, [22] 1.6, and observe that the Tychonoff cube is of negative type by the lemma above. For the second statement, embed M^n smoothly in some Euclidean space $\mathbb{R}^N$, and restrict the Euclidean distance to M^n. Then the result follows, modulo that $\mathbb{R}^N$ is of negative type. □

Excess matrices There is a useful characterization of negative type in terms of the excess function $e_{p,q}(r) = d(p, r) + d(r, q) - d(p, q)$:
For $Y = \{q_1, \dots, q_{|Y|}\} \subseteq X$ a finite ordered subset of X, define the excess matrix

$$\mathbf{E}_p(Y) := [e_{q_i,q_j}(p)] \in \mathrm{Sym}_{|Y|}(\mathbb{R}) \tag{4.4}$$

We have, cf. [13]:

Proposition 22. *Let X be a metric space. Consider the following conditions:*

1. *$\mathbf{E}_p(Y)$ is positive semidefinite for all finite ordered subsets Y.*

[1] see [23] for a discussion of Gromov-Hausdorff convergence

2. $\mathbf{E}_p(Y)$ *is positive definite for all finite ordered subsets* Y *with* $p \notin Y$.

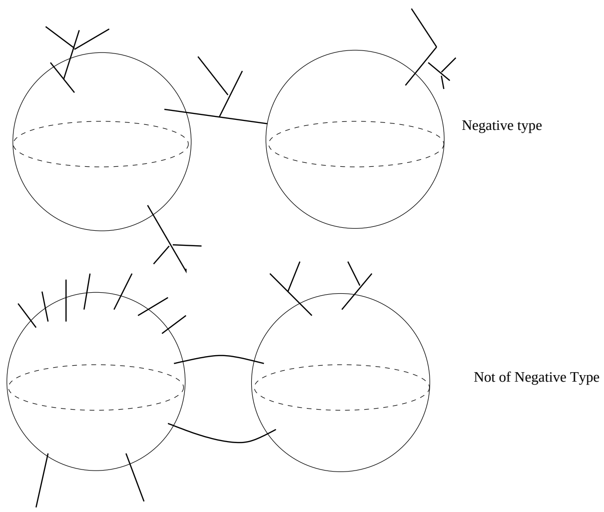
Then: there is a $p \in X$ *s.t. 1 is satisfied* $\iff$ *1 is satisfied for all* $p \in X$ $\iff$ $X \in \mathcal{NT}$. *The same holds when 1 is replaced by 2 and* $\mathcal{NT}$ *by* $\mathcal{SNT}$.

Recall that the one point union $Z = X \cup_p Y$ of two metric spaces is $Z = X \bigsqcup Y/\sim$, where two points $X \ni p_1 := p := p_2 \in Y$ are identified. The distance d_Z is defined such that $d_{Z|X} = d_X, d_{Z|Y} = d_Y$ and p is in between X and Y: $d_Z(x,y) := d_X(x,p) + d_Y(p,y)$ for $x \in X \subset Z, y \in Y \subset Z$. It is not difficult to see, that if X and Y are length spaces, then so is $X \cup_p Y$.

Corollary 5. *A one point union of two metric spaces* $Z = X \cup_p Y$ *is of (strictly) negative type iff* X *and* Y *are of (strictly) negative type.*

Proof. For any points $q \in X \subset Z$ and $r \in Y \subset Z$, we have by definition of the distance in $X \cup_p Y$ that $e_{q,r}(p) = 0$, p is in between X and Y. For any subset $W \subseteq Z$ we have: $W = U \cup V$ for some $U \subseteq X$ and $V \subseteq Y$ (and we may assume that p is contained in at most one of these). So (when W is finite) $\mathbf{E}_p(W)$ is a block matrix with $\mathbf{E}_p(U)$ and $\mathbf{E}_p(V)$ along the diagonal and zeroes elsewhere. $\square$

Figure 4.1: Two length spaces. The one on top is of negative type, while the bottom one is not. This will follow from the discussion in the remaining part of the thesis.



Proposition 23. *A metric space* X *on* 4 *points is of negative type, and of strictly negative type unless* X *consists of two pairs of antipodal points.*

Proof. The excess matrix $\mathbf{E}_p(X)$ with respect to some point $p \in X$, is a 3×3 symmetric matrix with positive entries such that the diagonal entry is dominant in each row (hence column) . The result follows by linear algebra (and some work…). $\square$

In table 4.1 some interesting spaces are divided according to type. $\mathbb{Q}$ denotes the quarternions, $\mathbb{CH}^n, \mathbb{QH}^n$ are the hyperbolic spaces over the complex numbers and the quarternions respectively, cf. [27]. $\mathbb{K}P^n$ denotes the projective spaces over $\mathbb{K}$. All results summarized in table 4.1 will be discussed in what follows.

Hypermetric	$\mathbb{M}(n, \kappa)$, 0-hyperbolic spaces
Strictly Negative Type	$\mathbb{CH}^n$, $\mathbb{M}(n, \kappa)$ for $\kappa \leq 0$, 0-hyperbolic spaces
Not of Negative Type	$\mathbb{QH}^n$, $\mathbb{K}P^n$ for $\mathbb{K} = \mathbb{R}, \mathbb{C}, \mathbb{Q}$ and $n \geq 2$

Table 4.1: Type of some interesting spaces ($\mathbb{Q}$ is the quarternions)

4.2 Type via Duality

Here we shall see that all 0-hyperbolic spaces and the Riemannian space forms $\mathbb{M}(n, \kappa)$ are hypermetric, and hence of negative type. The proofs uses a fundamental theorem of Kelly, see below, and the duality discussed previously. The classification according to strictly negative type, will be dealt with in section 4.4.

The main tool for proving hypermetricity is the following theorem of Kelly cf. [16] and [7] section 3.2 :

Theorem 8 (Kelly). *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space, then the semimetric on the set $\mathcal{A}$ of measurable subsets of Ω,*

$$d_\mu(A, B) := \mu(A \triangle B),$$

is hypermetric. Here $A \triangle B$ denotes the symmetric difference:

$$A \triangle B := A \cup B \setminus A \cap B$$

Corollary 6. *A 0-hyperbolic metric space is hypermetric, hence of negative type. The same holds for the space forms $\mathbb{M}(n, \kappa)$.*

Proof. Any finite subset of a 0-hyperbolic space is realizable in a finite weighted tree T, then the result follows from Kelly's Theorem by putting the dual measure on T (see section 2.6). The same holds for $\mathbb{M}(n, \kappa)$, the space forms are isometric to subsets of measure spaces (see the discussion in section 2.5). □

Example 11. By Kelly's Theorem, we have a finite hypermetric space associated to any finite subset $X \subset \mathbb{M}(n, \kappa)$, in the following curious way: For $p \in X$ define $V_p := \Delta(X \setminus \{p\})$, where Δ denotes the *convex hull*. This then gives a set associated to each point $p \in X$. Then we use the Riemannian volume form to get a measure and put $d(V_p, V_q) := \mathrm{vol}(V_p \triangle V_q)$. This off course also makes sense in more general settings. . .

4.3 Kernels, Mean Distance and Extent

Here we shall make use of measure and integration theory as in [22]. Hence from now on we assume that X is equipped with a topology which is sufficiently nice.

Definition 20. An *admissible* space (X, d) is a locally compact and separable metric space. An admissible *kernel* on X is a function $\phi : X \times X \to \mathbb{R}$, satisfying

1. $\phi(p, q) = \phi(q, p),\ \forall p, q \in X$ (symmetry)

2. ϕ is a Borel-function with respect to the product topology on $X \times X$.

3. ϕ is bounded on compact subsets of $X \times X$.

Unless otherwise mentioned, X is always assumed admissible (i.e. equipped with an admissible metric), and likewise for the kernel ϕ. Hence we will not consider electrostatic and gravitational potentials [2] like $\phi(x, y) = kd(x, y)^{\omega}$ for $\omega < 0$.

We are primarily interested in kernels of the form $f(d)$, when f is a continuous real function. In fact $f(d) = d$ is the situation we will have in mind most of the time, but (here) it doesn't hurt too much to treat things in a more general setting.

Generalities

Here some background material is presented. I must apologize for going a bit too much into tedious details, compared to the volume of applications covered later. But there are many more exciting applications than those presented in this thesis. And I found it difficult to find any standard reference covering the subject in a general setting. Hence it seemed necessary, at least for my own comfort, to go into some detail.

Measure theoretic terminology will be mostly as in [22], but we shall use the viewpoint of *Radon measures* on X instead of integrals; this makes no difference by the Riesz representation theorem. Notation will be a mix between notation in [22] and [1].

The set of (real) distributions, signed measures or *Radon charges* (as they are called in [22]) is the $\mathbb{R}$-span of all Radon measures on X. All such distributions can be decomposed as $\mu = \mu^+ - \mu^-$, where μ^+ and μ^- are positive Radon measures. We can choose the decomposition such that μ^+ and μ^- are concentrated on disjoint subsets:

$$Y^+ \cap Y^- = \emptyset,\ \mu^+(X \setminus Y^+) = 0 \text{ and } \mu^-(X \setminus Y^-) = 0, \tag{4.5}$$

c.f. [22] 6.5.7.

The norm or total absolute mass of μ is $\|\mu\| = |\mu|(X)$, where $|\mu|$ denotes the measure $\mu^+ + \mu^-$. The set of all distributions with finite norm will be denoted

$$\mathfrak{M}(X) := \{\mu \text{ a Radon charge with } \|\mu\| < \infty\}.$$

[2] Although such cases could be included with only a few extra technical complications...

The subset of $\mathfrak{M}(X)$ consisting of positive measures, i.e. $\mu = |\mu|$, will be denoted $\mathfrak{M}(X)^+$. That a Borel-function f is integrable with respect to a measure $\mu \in \mathfrak{M}^+$ is written $f \in \mathrm{L}^1(\mu)$. For $\mu \in \mathfrak{M}(X)$ and $f \in \mathrm{L}^1(|\mu|)$, $\int_X f\,\mu$ will mean $\int_X f\,\mu^+ - \int_X f\,\mu^-$.

The support of a distribution μ is the minimal closed set Y s.t. $|\mu|$ is concentrated on Y : $|\mu|(X \setminus Y) = 0$; it is denoted $\mathrm{supp}(\mu)$. δ_p will denote the Dirac measure with $\mathrm{supp}(\delta_p) = p$ and $\delta_p(p) = 1$. A nontrivial distribution in the span of a single Dirac measure $\mu = k\delta_p$, for $k \in \mathbb{R}^*$, will also be called an *atom*. The subset of distributions with compact support are denoted

$$\mathfrak{M}(X)_c := \{\mu \in \mathfrak{M}(X)|\ \mathrm{supp}(\mu) \text{ is compact }\} \tag{4.6}$$

The Banach space $\mathfrak{M}(X)$ is isometrically isomorphic to $(C_0(X))^*$, cf. Proposition 6.5.9 in [22]. Here $C_0(X)$ denotes the set of continuous function vanishing at infinity, that is $f \in C_0(X)$ iff $\{p \in X|\,|f(x)| > \epsilon\}$ is compact for all $\epsilon > 0$. We shall equip $\mathfrak{M}(X)$ with the w^*-topology (the weak topology):

$$\mu_n \to \mu \text{ iff } \int_X f\,\mu_n \to \int_X f\,\mu \text{ for all } f \in C_0(X)$$

The total algebraic mass of $\mu \in \mathfrak{M}(X)$ is $\mu(X) = \int_X 1\mu = \mu^+(X) - \mu^-(X)$, which is well defined since the positive measures μ^+, μ^- have finite mass.

Definition 21. We shall consider the following subsets of $\mathfrak{M}(X)$:

- $\mathfrak{atom}(X) := \{\mu \in \mathfrak{M}(X)|\ \mathrm{supp}(\mu) \text{ is a finite set}\}$
- $\mathfrak{B}(k) := \{\mu \in \mathfrak{M}(X)|\ \|\mu\| \le k\}$, for $k > 0$.
- $\mathfrak{S}(k) := \{\mu \in \mathfrak{M}(X)|\ \|\mu\| = k\}$, for $k > 0$.
- $\Pi_k(X) := \{\mu \in \mathfrak{M}(X)|\ \mu(X) = k\}$, for $k \in \mathbb{R}$.
- $\mathfrak{prop}(X) := \mathfrak{M}(X)^+ \cap \mathfrak{S}(1) = \Pi_1(X) \cap \mathfrak{B}(1)$

A distribution in $\mathfrak{prop}(X)$ is called a probability measure, and a distribution in the norm closure of $\mathfrak{atom}(X)$ is called atomic.

Notation 3. We shall use c as a subscript to denote that we consider the subset of distributions with compact support, e.g. $\Pi_k(X)_c := \Pi_k(X) \cap \mathfrak{M}(X)_c$.

Remark 17. $\mathfrak{B}(k)$ is always w^*-compact. For X a compact space also $\mathfrak{prop}(X)$ is w^*-compact, cf. 2.5.2 and 2.5.7. in [22]. $\mathfrak{S}(k)$ is not w^*-closed unless X is finite.

Clearly $\mathfrak{atom}(X)$ is a vector subspace of $\mathfrak{M}(X)$ and:

$$\mu \in \mathfrak{atom}(X) \iff \exists\{p_1, \ldots, \mathrm{p}_n\} \subset X, \alpha \in \mathbb{R}^n : \mu = \alpha_1\delta_{p_1} + \cdots + \alpha_n\delta_{p_n},$$

or written more compactly

$$\mathfrak{atom}(X) \cong \bigoplus_{p\in X} \mathbb{R}\delta_p$$

$\mathfrak{atom}(X)$ is not a closed subspace neither with respect to the weak topology or the norm topology, unless X is finite. In fact for X compact[3] $\mathfrak{atom}(X)$ is w^*-dense in $\mathfrak{M}(X)$. This follows from the Krein-Millman Theorem, c.f. [22] 2.5.8.

[3]Hence also for X σ-compact

Potentials and Quadratic forms

Given two distributions μ, ν on X let $\mu \otimes \nu$ denote the distribution on $X \times X$ s.t. $\mu \otimes \nu(U \times V) = \mu(U)\nu(V)$ for $U, V \subseteq X$. We will consider a kernel $\phi : X \times X \to \mathbb{R}$ as a quadratic form on (possibly a subset of) $\mathfrak{M}(X)$ by:

$$I(\mu, \mu) := \int\limits_{X \times X} \phi \quad \mu \otimes \nu :=$$

$$\int\limits_{X \times X} \phi \quad \mu^+ \otimes \mu^+ + \int\limits_{X \times X} \phi \quad \mu^- \otimes \mu^- - 2 \int\limits_{X \times X} \phi \quad \mu^- \otimes \mu^+ \tag{4.7}$$

However in order for this to make sense in general, we will have to restrict ourselves to distributions $\mu = \mu^+ - \mu^-$ such that ϕ is integrable with respect to the product measures appearing in (4.7). Since we only consider kernels that are bounded on compact subsets it is clear that the kernel is integrable wrt. all compactly supported distributions. A tensor product of two compactly supported distributions has compact support, since a product of compact sets is compact. We thus observe:

Observation 5. The compactly supported distributions on X are admissible in the sense that (4.7) gives a well defined quadratic/bilinear form on the vector space $\mathfrak{M}(X)_c$.

Potentials For a measure $\mu \in \mathfrak{M}(X)_c^+$ consider the expression:

$$\mathrm{p}_\mu(q) := \int_X \phi(p, q)\mu(p), \tag{4.8}$$

which means integration wrt. the variable p. By symmetry of ϕ it is irrelevant to keep track of which variable is “integrated away” to obtain p_μ.

p_μ is called the *potential* of μ, c.f. [1]. Given $\nu \in \mathfrak{M}(X)_c^+$, Fubini’s Theorem (in the very weak version [22] 6.6.4) ensures that

$$I(\mu, \nu) = \int_X \mathrm{p}_\mu \, \nu = \int_X \mathrm{p}_\nu \, \mu \tag{4.9}$$

This then extends to $\mu, \nu \in \mathfrak{M}(X)_c$ by bilinearity:

Definition 22 (Potential). Let X be an admissible space with an admissible kernel ϕ, and let $\mu = \mu^+ - \mu^- \in \mathfrak{M}(X)_c$. The function $\mathrm{p}_\mu : X \to \mathbb{R}$ is defined as:

$$\mathrm{p}_\mu(q) := \int_X \phi(p, q)\, \mu^+(p) - \int_X \phi(p, q)\, \mu^-(p), \tag{4.10}$$

and is called the potential of μ

Again Fubini ensures that for $\mu, \nu \in \mathfrak{M}(X)_c : I(\mu, \nu) = \int_X \mathrm{p}_\mu \, \nu = \int_X \mathrm{p}_\nu \, \mu$.

Terminology 3. The value $I(\mu,\mu)$ is called the *energy* of μ, and $I(\mu,\nu)$ the *mutual energy* of μ,ν.

Note that for an atom δ_p, we have $\mathrm{p}_{\delta_p}(q)=\phi(p,q)$. Hence in the case when ϕ is equal to the metric d we have:

$$\mathrm{p}_{\delta_p}=d(\cdot,p), \tag{4.11}$$

the distance from p.

Remark 18 (Restriction). In order to avoid unnecessary technical complications we shall restrict attention to the **compactly supported distributions**. The main application concerns compact subsets of Riemannian manifolds anyway. However it is possible to develop the entire theory allowing also distributions with non-compact support. Then one would restrict to a class of distributions larger than $\mathfrak{M}(X)_c$ such that (4.7) makes sense, and such that this set forms a vector space[4]

The lemma below follows from [22] 6.6.4.:

Lemma 13. *For $\mu\in\mathfrak{M}(X)_c$ we have: $\phi\in C(X\times X)\implies \mathrm{p}_\mu\in C(X)$, $\phi\in C_c(X\times X)\implies \mathrm{p}_\mu\in C_c(X)$, and $\phi\in C_0(X\times X)\implies \mathrm{p}_\mu\in C_0(X)$*

We then have the following basic, but important:

Lemma 14. *Let X be an admissible space with a continuous kernel ϕ and let $K\subseteq X$ be compact. If $\{\mu_n\}_{n\in\mathbb{N}}\subset\mathfrak{M}(K)\subseteq\mathfrak{M}(X)_c$ is a sequence converging weakly to $\mu\in\mathfrak{M}(K)$, then $\{\mathrm{p}_{\mu_n}\}_{n\in\mathbb{N}}$ converges uniformly to p_μ on every compact subset $C\subseteq X$.*

Proof. For simplicity assume that all distributions are positive measures in $\mathfrak{M}(K)^+$. Since K is compact and $\mu_n\to\mu:=\mu_\infty$ weakly in $\mathfrak{M}(K)^+$, we have $\mu_n(K)\to\mu(K)$. Hence the set $\{\mu_n(K)\}_{n\in\hat{\mathbb{N}}}$ is bounded by some constant $b<\infty$ (here $\hat{\mathbb{N}}:=\mathbb{N}\cup\{\infty\}$). But then for any compact subset C, the set of functions $\{\mathrm{p}_{\mu_n}\}_{n\in\hat{\mathbb{N}}}$ forms an *equicontinuous* family of functions on C:

$$|\mathrm{p}_{\mu_n}(p)-\mathrm{p}_{\mu_n}(q)|\le\int_K|\phi(p,r)-\phi(q,r)|\mu_n(r)\le b\sup_{r\in K}\{|\phi(p,r)-\phi(q,r)|\},$$

for $n\in\hat{\mathbb{N}}$. Then equicontinuity follows from uniform continuity of ϕ on $C\times K$.

Since $\mu_n\to\mu$ weakly in $\mathfrak{M}(K)^+$, then simply by definition of weak convergence $\{\mathrm{p}_{\mu_n}\}$ converges pointwise to $\mathrm{p}_{\mu_\infty}=\mathrm{p}_\mu$ on X. Now for every $\epsilon>0$ there is a $\delta>0$ such that $d(p,q)\le\delta\implies|\mathrm{p}_{\mu_n}(p)-\mathrm{p}_{\mu_n}(q)|<\epsilon$ for all $n\in\hat{N}$. Then we may choose a finite δ-net $\{p_1,\dots,p_m\}\subseteq C$, and $n_0\in\mathbb{N}$ such that $n>n_0$ implies $|\mathrm{p}_{\mu_n}(p_i)-\mathrm{p}_\mu(p_i)|<\epsilon$ for $i=1\dots m$. But it is easy to see that this implies $|\mathrm{p}_{\mu_n}(p)-\mathrm{p}_\mu(p)|<3\epsilon$ for all $p\in C$. □

[4] which is the case precisely when $\phi\in\mathrm{L}^1(|\mu|\otimes|\mu|)\cap\mathrm{L}^1(|\nu|\otimes|\nu|)\implies\phi\in\mathrm{L}^1(|\mu|\otimes|\nu|)$. This happens e.g. for positive kernels where an inequality of the form $\phi(x,y)\le k(\phi(x,z)+\phi(z,y))$ or $\phi(x,y)\le k(\phi(x,z)\phi(z,y))$ gives a separation of the variables. Examples are d^γ,$\exp(d)$ and $\cosh(d)$.

The following lemma is fundamental:

Lemma 15. *Let X be an admissible space with kernel ϕ*

$$\mathfrak{M}(X)_c \ni \mu \mapsto I(\mu,\mu) \tag{4.12}$$

is norm continuous iff ϕ is bounded and w^*-continuous iff $\phi \in C_0(X \times X)$.

Proof. The first statement is easy. Here we will just prove that X compact implies that the quadratic form is w^*-continuous, the extension to X noncompact is not difficult.

So let X be compact and ϕ a continuous kernel. Assume that $\mu_n \to \mu$ weakly. Then $\mathrm{p}_{\mu_n} \to \mathrm{p}_\mu$ uniformly on X by the previous lemma. We have

$$\textstyle\int_X \mathrm{p}_\mu\,\mu - \int_X \mathrm{p}_\mu\,\mu + \int_X (\mathrm{p}_\mu - \mathrm{p}_{\mu_n})\,\mu_n \to 0,$$

because $\{\mu_n(X)\}$ is bounded. But we also have $\int_X \mathrm{p}_\mu\,\mu - \int_X \mathrm{p}_\mu\,\mu_n \to 0$ by weak convergence. Hence rearranging we see:

$$I(\mu,\mu) - I(\mu_n,\mu_n) = \int_X \mathrm{p}_\mu\,\mu - \int_X \mathrm{p}_{\mu_n}\,\mu_n \to 0$$

□

Example 12. A Radon charge on a finite set $X = \{p_1, \ldots, p_n\}$ is nothing but a distribution of masses, i.e. a vector $\mu = (x_1, \ldots, x_n) \in \mathbb{R}^n$. $\mathfrak{M}(X)$ is then identified with $\mathbb{R}^n$ equipped with the l_1-norm. The total algebraic mass is $\mu(X) = \sum_{i=1}^n x_i$, while the integral of a function $\phi : X \times X \to \mathbb{R}$ is $\sum_{i,j} x_i x_j \phi(p_i, p_j)$.

The potential of $\mu = (x_1, \ldots, x_n)$ can be seen as the linear form $\nu \mapsto \nu^t \mathbf{M}_\phi \mu$, where μ, ν are considered as column vectors and $\mathbf{M}_\phi := [\phi(p_i, p_j)] \in \mathrm{Sym}_n\,\mathbb{R}$ is the matrix of ϕ. The map $\mu \mapsto \mathrm{p}_\mu$ is then injective iff $\mathbf{M}_\phi \in \mathrm{Gl}_n(\mathbb{R})$.

Extremal energies and their realizations

Definition 23. Let X be an admissible space with kernel ϕ. Define the following numbers in $\mathbb{R} \cup \{\infty\}$:

$$I_k(X,\phi) := \sup\{I(\mu,\mu) \mid \mu \in \Pi_k(X)_c\}$$

$$\mathrm{nt}(X,\phi) := \sup\{I(\mu,\mu) \mid \mu \in \Pi_0(X)_c \cap \mathfrak{S}(2)\}$$

$$\mathrm{xt}(X,\phi) := \sup\{I(\mu,\mu) \mid \mu \in \mathfrak{prop}(X)_c\}$$

Observation 6. Considering the kernel $-\phi$ we have $I_{-\phi} = -I_\phi$, and we get $\mathrm{xt}(X,-\phi) = \inf\{I_\phi(\mu,\mu) \mid \mu \in \mathfrak{prop}(X)_c\}$ etc.

Remark 19 (Probabilistic interpretation). Given $\mu, \nu \in \mathfrak{prop}(X)_c$ we have the following probabilistic interpretation: $I(\mu,\nu)$ is the expectation value of $\phi(x,y)$ when the first coordinates are randomly distributed according to μ and second coordinate points are distributed independently according to ν. We see that $\mathrm{xt}(X,\phi)$ is the maximal expectation value when the two coordinates (stochastic variables) have the same distribution.

If $\mathrm{nt}(X,\phi) > 0$ then by scaling it is clear that $I_0(X,\phi) = \infty$, hence not realized in $\Pi_0(X) \cap \mathfrak{M}(X)_c$.

Proposition 24. *Let X be a compact admissible space with continuous kernel ϕ.*

- *There is a probability measure realizing* $\mathrm{xt}(X,\phi)$.
- *If* $\mathrm{nt}(X,\phi) < 0$ *then X is finite and the supremum is realized.*
- *If* $\mathrm{nt}(X,\phi) > 0$ *then the supremum is realized.*

Proof. When X is compact the map $\mu \mapsto \mu(X)$ i.e. taking total algebraic mass is w^*-continuous since $\mu(X) = \int_X 1\,\mu$. Hence the sets $\Pi_k(X)$ are weakly closed. It follows that $\mathfrak{prop}(X) = \Pi_1(X) \cap \mathfrak{B}(1)$ and also $\Pi_0(X) \cap \mathfrak{B}(2)$ are w^*-compact. The map $\mu \mapsto I(\mu,\mu)$ is weakly continuous since ϕ is continuous on $X \times X$, c.f. Lemma 15. Then the sup is realized on $\mathfrak{prop}(X)$, which settles the first case.

Suppose that $\mathrm{nt}(X,\phi) < 0$. We have $\mu = (\delta_p - \delta_q) \in \Pi_0(X) \cap \mathfrak{S}(2)$ for all $p \neq q$ and $I(\mu,\mu) = \phi(p,p) + \phi(q,q) - 2\phi(p,q)$. This converges to zero for a sequence $p_n \to q$ s.t. $p_n \neq q$. We always have such sequences unless X is discrete, hence compact iff X is finite. If X is finite the sup is realized by compactness of $\mathfrak{S}(2)$. So if X is not finite, then we must have $\mathrm{nt}(X,\phi) \geq 0$.

On $\Pi_0(X) \cap \mathfrak{B}(2)$ the sup is realized, and this sup is not less than the one taken over $\Pi_0(X) \cap \mathfrak{S}(2) \subset \Pi_0(X) \cap \mathfrak{B}(2)$. So if $\mathrm{nt}(X) > 0$ this is also the case for the sup realized in $\Pi_0(X) \cap \mathfrak{B}(2)$. But the distribution μ realizing this must be nontrivial. So by multiplying μ with $\frac{2}{\|\mu\|}$ we obtain an element $\tilde{\mu} \in \Pi_0(X) \cap \mathfrak{S}(2)$, which must have larger energy $I(\tilde{\mu},\tilde{\mu}) = \frac{4}{\|\mu\|^2} I(\mu,\mu) > I(\mu,\mu)$, unless $|\mu\| = 2$. Hence μ must actually be an element in $\Pi_0(X) \cap \mathfrak{S}(2)$. $\square$

Definition 24. Let X be an admissible space with a kernel ϕ, and let $\mathfrak{V}$ be a subspace of $\mathfrak{M}(X)_c$.

ϕ is defined to be of $\mathfrak{V}$-negative type iff $I(\mu,\mu) \leq 0$ for all $\mu \in \Pi_0(X) \cap \mathfrak{V}$, and of strictly $\mathfrak{V}$-negative type iff $I(\mu,\mu) < 0$ for all $\mu \in \Pi_0(X) \cap \mathfrak{V} \setminus \{0\}$.

The following shows the importance of strictly negative type:

Proposition 25. *If ϕ is of strictly $\mathfrak{V}$-negative type and $\mu \in \mathfrak{V}$ realizes either* $\mathrm{xt}(X,\phi)$ *or $I_k(X,\phi)$, then μ is the unique realization in $\mathfrak{V}$. If ϕ is only of $\mathfrak{V}$-negative type, then any convex linear combination of two realizations is again a realization.*

Proof. Suppose that two distributions $\mu_0, \mu_1 \in \mathfrak{V}$ realize one of the sup's. Then $\nu = \mu_1 - \mu_0 \in \Pi_0(X) \cap \mathfrak{V}$ and by convexity $\mu_t = \mu_0 + t\nu$ defines a distribution in one of the relevant subsets for $t \in [0,1]$. Then:

$$I(\mu_t,\mu_t) = I(\mu_0,\mu_0) + 2tI(\mu_0,\nu) + t^2 I(\nu,\nu) \tag{4.13}$$

But if ν is non trivial and we have strictly $\mathfrak{V}$-negative type, then $I(\nu,\nu) > 0$ and μ_0 is clearly not a maximum. Hence $\mu_0 = \mu_1$. In case we only have $\mathfrak{V}$-negative type, we can conclude that $I(\nu,\nu) = I(\mu_0,\nu) = 0$. Hence for any $t \in [0,1]$, $\mu_0 + t\nu$ is also a realization. $\square$

Note that the previous definition of negative type and strictly negative type, Definition 19, is exactly the same as $\mathfrak{atom}(X)$-negative/strictly negative type of the distance kernel $\phi = d$, as defined above.

Remark 20 (Physical Interpretation). Viewing $I(\mu, \mu)$ as an energy, strictly $\mathfrak{V}$-negative type, means that whenever we have a distribution in $\mathfrak{V}$, with total mass zero, the energy is strictly negative. Hence the configuration cannot collapse, with negative and positive mass canceling out, since the zero distribution has larger energy.

If we consider the distance kernel d, then atoms of same sign attract each other, since the energy increases with distance, while atoms of opposite sign repulse each other. Then strictly negative type means that an atomic configuration with zero total mass has strictly negative energy. If the space X is noncompact such a configuration is likely to diverge to infinity. While if X is compact it is easily seen that the minimum energy is attained when atoms of same sign join up in two piles at points realizing $\operatorname{diam}(X)$.

Reversing the sign, considering the kernel $-d$, the interpretation is reversed and the situation looks more familiar. Same sign atoms repulse and opposite sign atoms attract. If X is of strictly negative type (and is not discrete) the minimal energy is zero and the configuration will be likely to collapse and mass cancel out. If X is not of negative type, then the minimal energy is (bounded by) $-\operatorname{nt}(X, d) < 0$ and the configuration could thus find a stable equilibrium.

Lemma 16. *Let X be an admissible space with kernel ϕ.*

- *If $\mu \in \Pi_k(X)_c$ realizes $I_k(X, \phi)$ for some $k \in \mathbb{R}$, then $I(\mu, \nu) = 0$ for all $\nu \in \Pi_0(X)_c$, which means that p_μ is a constant function.*
- *If $\mu \in \Pi_0(X)_c \cap \mathfrak{S}(2)$ realizes $\operatorname{nt}(X, \phi)$, then $I(\mu, \nu) \leq 0$ for any $\nu \in \Pi_0(X)_c$ such that $\|\mu + \epsilon\nu\| \leq 2$ for ϵ sufficiently small.*
- *If μ realizes $\operatorname{xt}(X, \phi)$, then $I(\mu, \nu) \leq 0$ for any $\nu \in \Pi_0(X)_c$ such that $\mu + \epsilon\nu \in \mathfrak{prop}(X)_c$ for ϵ sufficiently small.*

Proof. All statements follow by analyzing the quadratic expression:

$$I(\mu + \epsilon\nu, \mu + \epsilon\nu) = I(\mu, \mu) + \epsilon^2 I(\nu, \nu) + 2\epsilon I(\mu, \nu), \tag{4.14}$$

and observing that the last term, if nonzero, is dominant for $\epsilon \to 0$. That $I(\mu, \nu) = \int_X p_\mu \, \nu = 0$, for all $\nu \in \Pi_0(X)_c$ means by putting $\nu = \delta_p - \delta_q : \int_X p_\mu \nu = \mathrm{p}_\mu(p) - \mathrm{p}_\mu(q) = 0$, hence p_μ is constant. $\square$

An important property is that in an admissible space with a continuous kernel the integral $I(\mu, \mu)$, for $\mu \in \mathfrak{M}(X)_c$, can be approximated by a sequence of integrals of atomic measures having the same amount of positive and negative mass as μ.

Lemma 17. *Let X be an admissible space with a continuous kernel ϕ and let $\mu \in \mathfrak{M}(X)_c$. For every $\epsilon > 0$ there is a finitely supported distribution $\mu_A \in \mathfrak{atom}(X)$ s.t.:*

$$|I(\mu, \mu) - I(\mu_A, \mu_A)| < \epsilon \text{ with } \mu^+(X) = \mu_A^+(X),\ \mu^-(X) = \mu_A^-(X)$$

Proof. The analysis restricts to the compact set $K = \operatorname{supp}(\mu)$. Put $k_1 = \mu^+(K)$ and $k_2 = \mu^-(K)$. By w^*-density of $\mathfrak{atom}(K)$ in $\mathfrak{prop}(K)$, c.f. Remark 17, we can find sequences of positive measures $\{\mu_n^+\} \subset \mathfrak{S}(k_1) \cap \mathfrak{atom}(K)$ and $\{\mu_n^-\} \subset \mathfrak{S}(k_2) \cap \mathfrak{atom}(K)$, s.t. $\mu_n^+ \to \mu^+$ and $\mu_n^- \to \mu^-$ weakly for $n \to \infty$. Since μ^+ and μ^- are concentrated on disjoint subsets of K, we can furthermore choose the sequences such that μ_n^+ and μ_n^- are concentrated on disjoint subsets. The result now follows from w^*-continuity of $\nu \mapsto I(\nu, \nu)$ on $\mathfrak{M}(K)$, Lemma 15. $\square$

Theorem 9. *Let X be an admissible space with a continuous kernel ϕ. The following statements are equivalent:*

1. (X, ϕ) *is of* $\mathfrak{M}(X)_c$*-negative type*
2. (X, ϕ) *is of negative type (i.e.* $\mathfrak{atom}(X)$*-negative type)*
3. $\operatorname{nt}(X, \phi) \leq 0$
4. $I_0(X, \phi) \leq 0$

Proof. 1 implies 2 by definition, since $\mathfrak{atom}(X) \subseteq \mathfrak{M}(X)_c$. 2 $\Longrightarrow$ 1 follows from Lemma 17. 3 and 4 are clearly equivalent to 1 (by scaling in the case of 3). $\square$

4.4 First Applications

We shall give some first applications using Lemma 16; most of these results can be strengthened. Here we just want to show how easily the potential formulation can be applied to deduce interesting results.

Proposition 26. *Let X be a manifold with a kernel ϕ which satisfies:*

$$\phi \in C^m(X \times X \setminus \mathcal{D}, \mathbb{R}), \ \text{where } \mathcal{D} := \{(p, p) | \, p \in X\}, \tag{4.15}$$

for some $m \in \mathbb{N}_0$, and assume that ϕ is not of class C^m on any neighborhood intersecting the diagonal $\mathcal{D}$. Then $I_k(X, \phi)$ is not realized by a finitely supported distribution if $k \neq 0$ and $I_0(X, \phi)$ is not realized by any nontrivial finitely supported distribution.

Proof. Suppose $\mu \in \Pi_k(X) \cap \mathfrak{atom}(X)$ realizes $I_k(X, \phi)$, then p_μ is constant by Lemma 16. Since we assume that μ is nontrivial, we must have that $|\operatorname{supp}(\mu)| > 2$, because otherwise ϕ must be constant. But then:

$$\mu = \sum_{i=1}^{n} \alpha_i \delta_{p_i} \implies \mathrm{p}_\mu = \sum_{i=1}^{n} \alpha_i \phi(\cdot, p_i) \tag{4.16}$$

However constancy of this would imply, for any i, that $\phi(\cdot, p_i)$ is C^m also at p_i. $\square$

Then we have, when specializing to the case $I_0(X, d)$:

Corollary 7. *An Hadamard manifold X whose distance kernel is of negative type is also of strictly negative type. Hence $\mathbb{M}(n,\kappa) \in \mathcal{SNT}$ for $\kappa \leq 0$.*

Proof. In an Hadamard (c.f. [5] or [21]) manifold, the distance is smooth away from the diagonal, hence the result follows from the proposition above. $\square$

Remark 21. This does give a much easier argument for the fact, that the space forms $\mathbb{M}(n,\kappa)$ are of strictly negative type, than the one given in [14]. We do not need to know any specifics about the variation to get the conclusion from Lemma 16 that p_μ is constant for a realization of $I_k(X,\phi)$. Also note that we do not need any $\mathfrak{M}(X)$-theory to get the conclusions above: Lemma 16 is completely valid if we restrict attention only to the finitely supported distributions $\mathfrak{atom}(X)$.

Corollary 8. *For $\mathbb{M}(n,0) = \mathbb{R}^n$, the modified distance kernel d^ω is of strictly negative type if $\omega \in [0,2)$*

Proof. It is known that for the Euclidean spaces $\mathbb{R}^n = \mathbb{M}(n,0)$ the modified distance d^ω is a kernel of negative type for $\omega \in [0,2]$, c.f. [7]. This follows from the fact that d^2 is a kernel of negative type, which is easy to see from the excess matrix criterion of Proposition 22. But one can show by basic means, that modification of a kernel as $\phi \mapsto \phi^\omega$ preserves negative type for $\omega \in [0,1]$.

Then it follows from Proposition 26 that $I_0(\mathbb{R}^n, d^\omega) = 0$ is not realized by a finitely supported distribution since for $\omega < 2$, d^ω is smooth away from the diagonal but not C^2 on the diagonal. Here we use the interpretation that 0^0 is 0, when $\omega = 0$. $\square$

In [8] it is shown that the distance kernel on $\mathbb{CH}^n$, complex hyperbolic space, is of negative type, hence we have:

Corollary 9. *$\mathbb{CH}^n \in \mathcal{SNT}$ for all $n \in \mathbb{N}$.*

Complex hyperbolic space is then an example of an interesting space of *nonconstant* curvature, but highly symmetric though, which is of strictly negative type. The first impulse is then to think that quarternionic hyperbolic spaces would also be of negative type, and perhaps this would be true for all Hadamard manifolds? However negative type of $\mathbb{QH}^n$ can be excluded by a property of the isometry group of these spaces. See [26] and [27], which contains further references on this.

The argument in the case of Hadamard manifolds has a counterpart for *geometrized trees*, c.f. section 2.6.

Proposition 27. *Let $\tilde{T}$ be a geometrized weighted tree, which contains at least one branch point, then $I_k(\tilde{T}, d)$ is not realized by any finitely supported nontrivial distribution.*

Proof. Let μ be a distribution in $\Pi_k(\tilde{T}) \cap \mathfrak{atom}(\tilde{T})$, which we may assume contains at least two atoms. For any point $p \in \tilde{T}$ contained in the interior of a 1-simplex $\tilde{e}$, p divides $\tilde{T}$ into two disjoint open sets $\tilde{T}^+$ and $\tilde{T}^-$. Let γ be a geodesic through p, which we parametrize such that $\gamma(t) \in \tilde{T}^+$ for $t > 0$. If $\mu(p) = 0$, we then clearly have $\frac{d}{dt}\mathrm{p}_\mu(\gamma(t)) = \mu(\tilde{T}^+) - \mu(\tilde{T}^-)$, for $t > 0$ so small that $\gamma([0,t]) \cap \mathrm{supp}(\mu) = \emptyset$. This derivative must be zero for all such p if p_μ is constant, which implies that there should be equal mass on "both sides" of p. But this is clearly impossible unless $\tilde{T}$ is an interval with an atom in each end. $\square$

Corollary 10. *All* 0*-hyperbolic spaces are of strictly negative type.*

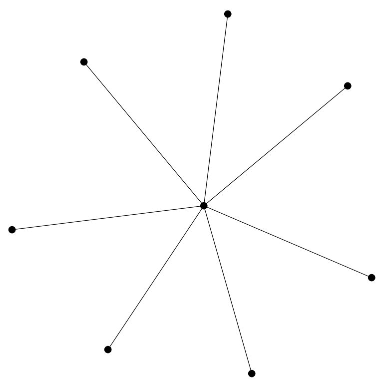
Proof. Any finite subset X of a 0-hyperbolic space is realizable in a geometrized tree $\tilde{T}$. Hence a nontrivial realization of $I_0(X, d) = 0$ would also be a realization of $I_0(\tilde{T}, d)$; impossible by the previous result. $\square$

For a *leaf space* the above result already follows from the fact that $\mathbb{H}(n, \kappa)$ is of strictly negative type, and that $X \overset{isom}{\hookrightarrow} \mathbb{H}(n, \kappa)$ for some n, and $|\kappa|$ large enough.

In between the two extremes, *Hadamard manifolds* and *weighted trees*, there are a lot of other simply connected length spaces of nonpositive curvature, for which similar techniques should apply.

Star Spaces, an example

Figure 4.2: A geometrized star graph



Here we will give an example illustrating some of the introduced concepts. Recall from chapter 3, that a regular n-star graph $\mathrm{Star}(n, \frac{1}{2})$ is a graph $G = (V, E, w)$ with one vertex of degree n and n vertices of degree 1. The edges has length $\frac{1}{2}$, hence the diameter is 1. Geometrizing the graph, i.e. considering it as a 1-dimensional simplicial complex, is the same thing as gluing n copies of $[0, \frac{1}{2}]$ together by identifying left endpoints. This space $\widetilde{\mathrm{Star}}(n, \frac{1}{2})$ is then a compact, 0-hyperbolic space with the path metric d.

From Proposition 24 we know that there is a probability μ measure realizing $\mathrm{xt}(\widetilde{\mathrm{Star}}(n, \frac{1}{2}), d)$. We shall give an argument later of the somewhat obvious fact, that this

μ can only have support at the boundary points, the *leaves*. Hence μ is atomic, and since we have strictly negative type the realization is unique. But then by symmetry of the leaves we must have $\mu(l_i) = \frac{1}{n}$, μ has an atom of mass $\frac{1}{n}$ at each leaf. A calculation gives:

$$\mathrm{xt}(\mathrm{Star}(n, \frac{1}{2})) = 2\binom{n}{2}\frac{1}{n^2} = \frac{n(n-1)}{n^2}$$

We could also consider a star graph with countably many leaves, which is not compact but an admissible space anyhow. Then clearly $\mathrm{xt}(\mathrm{Star}(\infty, \frac{1}{2})) = 1$, but the extent is not realized.

If we go to the extreme we could consider a star with uncountably many leaves. This would not be an admissible space in itself. However we could consider an uncountable star parameterized by e.g. $[0, 1]$: Define a kernel ϕ on $[0, 1]$, such that $\phi(x, y) = 1$ for $x \neq y$ and $\phi(x, x) = 0$ for all $x, y \in [0, 1]$. Then ϕ is a 0-hyperbolic metric on $[0, 1]$ and is of strictly negative type. However it is easily seen that ϕ is not of strictly $\mathfrak{M}([0, 1])$-negative type [5] (since any continuous distribution realizes $\mathrm{xt}(X, \phi) = 1$).

4.5 Geometric Significance

Here we will consider geometric interpretation of the concepts introduced, especially try to get a grasp on what negative type means. So let's restrict attention to the most geometrically relevant situation when the kernel is d, *the metric defining the topology*. However all that follows will make sense for a kernel which is a continuous metric (or just a distance in some results). When the kernel is d, we will just write $\mathrm{xt}(X)$ instead of $\mathrm{xt}(X, d)$, etc.

Mean Distance

Definition 25 (Mean Distance). Let (X, d) be an admissible space. For two compact subsets $U, V \subseteq X$ and fixed measures $\mu \in \mathfrak{prop}(U) \subseteq \mathfrak{M}(X)_c$, $\nu \in \mathfrak{prop}(V) \subseteq \mathfrak{M}(X)_c$ define the mean distance wrt. $\mu_1 \otimes \mu_2$:

$$\mathrm{md}(U, V) := I(\mu_1, \mu_2) = \int_{U \times V} d \quad \mu_1 \otimes \mu_2 \tag{4.17}$$

For $U = V$ and $\mu_1 = \mu_2$ we write $\mathrm{md}(U) := \mathrm{md}(U, U) = I(\mu, \mu)$.

Writing $\mathrm{md}(\mu, \nu)$ for $\mu, \nu \in \mathfrak{M}(X)_c$ would perhaps be more clear. However $\mathrm{md}(U, V)$ for some μ, ν with $\mathrm{supp}(\mu) \subseteq Y$ and $\mathrm{supp}(\nu) \subseteq X$ seems more geometrical. Whenever

[5] This does raise the question: When does strictly $\mathfrak{atom}(X)$-negative type imply strictly $\mathfrak{M}(X)_c$-negative type? Is continuity of ϕ enough? Note that if we have continuity of ϕ and X is compact, then $\mu \mapsto \mathrm{p}_\mu \in C(X)$ is w^*-continuous, hence the kernel is w^*-closed. The answer is probably trivial among measure theorists…

important, the specific measures, which do not appear in notation, will be clear from context.

With this terminology it is sensible to think of the potential p_μ of a distribution $\mu \in \mathfrak{M}(X)_c$ with respect to the distance kernel d, as the *mean distance function* to $\mathrm{supp}(\mu)$. For $q \notin \mathrm{supp}(\mu)$, we can also think of $\mathrm{p}_\mu(q)$ as the distance to the "center of mass", defined as a minimum point of p_μ. However this terminology is probably more relevant, when we consider the potential of a modification of the distance kernel. e.g. $f(d) = d^2$ on $\mathbb{R}^n$.

Extent Also it makes sense to say that $\mathrm{xt}(X) = \sup\{\mathrm{md}(X, X) | \mu \in \mathfrak{M}(X)\}$ is the *maximal mean distance,* which is finite and realized when X is compact.

In [10],[13], the q-extent of a compact metric space is defined as:

$$\mathrm{xt}_q(X) := \max\{\mathrm{xt}_q(p_1, \ldots, p_q) | (p_1, \ldots, p_q) \in X^q\}, \tag{4.18}$$

where

$$\mathrm{xt}_q(p_1, \ldots, p_q) := \frac{1}{2}\binom{q}{2}^{-1} \sum_{i,j=1}^{q} d(p_i, p_j), \tag{4.19}$$

and X^q is short for $X \times X \times \cdots \times X$, q times. So $\mathrm{xt}_q(X)$ is the maximal mean distance in q-tuples of points (and this is realized by compactness). The factor of $\frac{1}{2}$ in (4.19) is due to our convention on summing all pairs twice. We have $\frac{1}{2}\binom{q}{2}^{-1} = \frac{1}{q(q-1)}$. The extent of X is then defined in [10] and [13] as:

$$\mathrm{xt}_{GM}(X) := \lim_{q\to\infty} \mathrm{xt}_q(X) \tag{4.20}$$

But the sum in (4.19) may be seen as the integral of d with respect to a positive atomic measure with atoms at p_i, $i = 1 \ldots q$, and total mass $\frac{q}{\sqrt{q(q-1)}} = q w_q$, where each element of the tuple $(p_1, \ldots, p_q)$ has weight equal to w_q. This can be written explicitly as:

$$\begin{gathered} x = (p_1, \ldots, p_q) \in X^q \sim \mu_x := \textstyle\sum_{i=1}^q w_q \delta_{p_i} \implies \\ \mathrm{xt}_q(p_1, \ldots, p_n) = \int_{X\times X} d \quad \mu_x \otimes \mu_x \end{gathered}$$

A point p can appear many times in the tuple, $p = p_{i_1} = p_{i_2} \ldots$, hence the resulting mass of the atom at p may be larger than w_q.

Since the total mass of μ_x is less than 1, we have $\mathrm{xt}_q(X) < \mathrm{xt}(X)$ for all q, hence $\mathrm{xt}_{GM} \leq \mathrm{xt}(X)$. But by Lemma 17, we can approximate $\mathrm{xt}(X)$ arbitrarily using an atomic probability measure μ_A, which again can be approximated by q-tuples as above: choose q so large and p so many times that $(\#p)w_q = \frac{\#p}{\sqrt{q(q-1)}}$ is close to $\mu_A(p)$, where $\#p$ is number of times p appears in the q-tuple. We then have:

Proposition 28. *Let X be a compact metric space, then* $\mathrm{xt}_{GM}(X) = \mathrm{xt}(X)$

Hence we may refer to [10] for properties of the extent invariant for compact Alexandrov spaces.

Example 13 (Mean distance and extent of an interval). What is the expectation value of the (usual) distance when points are chosen randomly with uniform distribution on the interval [0, 1]? Uniform means here, that we consider the Lebesgue measure. An easy calculation gives:

$$\mathrm{md}([0,1]) = \int_0^1 \int_0^1 |x-y|\, dx dy = \frac{1}{3} \tag{4.21}$$

We also know from Proposition 24 that there is a probability measure $\mu \in \mathfrak{prop}([0,1])$ realizing xt([0, 1]), the maximal mean distance. This μ is obtained by placing an atom of mass $\frac{1}{2}$ in both "ends", i.e. $\mu = \frac{1}{2}(\delta_0 + \delta_1)$; as follows from [1]. A calculation gives $\mathrm{xt}([0,1]) = \frac{1}{2}$.

Calculating the mean distance with respect to Lebesgue measure of higher dimensional sets turns out to be quite difficult, in fact impossible by direct methods.

Figure 4.3: The potential of Lebesgue measure on [0, 1]. We get a subharmonic, but not smooth function!

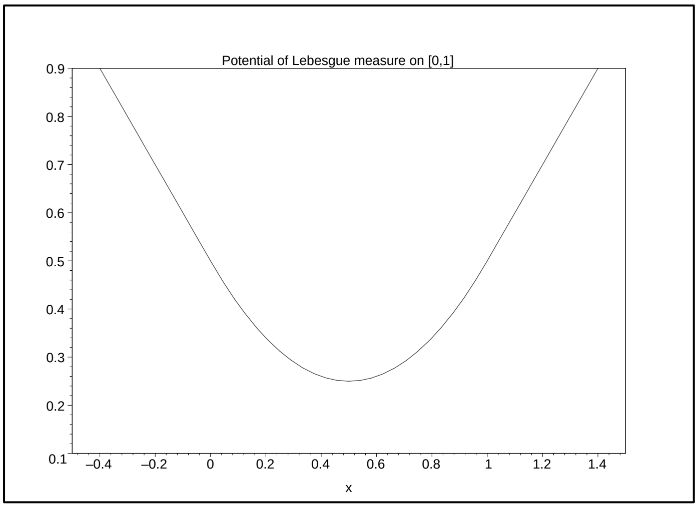
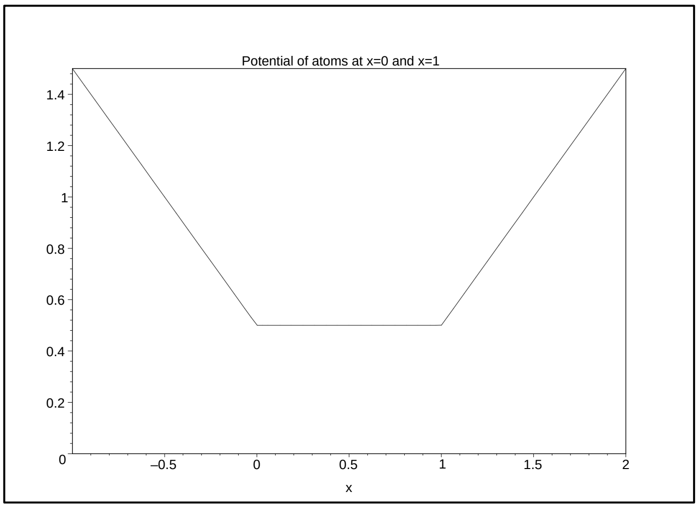


Figure 4.4: Potential of the measure realizing xt([0, 1])



Geometric Characterizations of Negative Type

Here is a more geometrically appealing characterization of negative type:

Proposition 29. *Let X be an admissible space. d is of negative type if and only if: For all compact $U, V \subseteq X$ and all probability measures on these:*

$$\mathrm{md}(U) + \mathrm{md}(V) \leq 2\,\mathrm{md}(U, V), \tag{4.22}$$

or equivalently:

$$\mathrm{md}(U, V) \geq \frac{\mathrm{md}(U) + \mathrm{md}(V)}{2} \tag{4.23}$$

Proof. Assume d is of negative type, hence $\mathfrak{M}(X)_c$-negative type. Let $\mu \in \mathfrak{prop}(U)$, $\nu \in \mathfrak{prop}(V)$. Then observe that $\mu - \nu \in \Pi_0(X)_c$ and (4.22) is simply a rewriting of $I(\mu - \nu, \mu - \nu) \leq 0$.

Conversely given $\mu \in \Pi_0(X)_c$ put $U = \mathrm{supp}(\mu^+)$ and $V = \mathrm{supp}(\mu^-)$ and scale μ such that $\|\mu\| = 2$ (assuming $\mu \neq 0$). Then again (4.22) gives $I(\mu, \mu) = I(\mu^+ - \mu^-, \mu^+ - \mu^-) \leq 0$. $\square$

As in Remark 19, we can give (4.23) a probabilistic interpretation: choosing points randomly in U according to a fixed probability distribution, and independently in V with another distribution, the mean of the expectation values of distances in U and distances in V is less than the expectation value of distances between U and V.

The following is a couple of elementary observations, which should help the geometric intuition a bit:

Proposition 30. *Let (X, d) be an admissible space, and put*

$$d(U, V) := \inf_{p \in U, q \in V} \{d(p, q)\} \tag{4.24}$$

for compact $U, V \subset X$.

- *Suppose $d(U, V) \geq \frac{1}{2}(\mathrm{diam}(U) + \mathrm{diam}(V))$. Then for any probability measures on U, V : $\mathrm{md}(U) + \mathrm{md}(V) \leq 2\,\mathrm{md}(U, V)$.*
- $\mathrm{md}(U, W) \leq \mathrm{md}(U, V) + \mathrm{md}(V, W)$, *for compact subsets $U, V, W \subseteq X$ and any probability measures on these.*

More interesting is:

Theorem 10. *Let (X, d) be a compact metric space on more than one point. Then*

- $\frac{1}{2}\,\mathrm{diam}(X) \leq \mathrm{xt}(X) < \mathrm{diam}(X)$
- *If X is of negative type then*

$$\mathrm{xt}(X) = \frac{1}{2}\,\mathrm{diam}(X) \iff \mathrm{exc}(X) = 0 \tag{4.25}$$

Proof. Let p and q be such that $d(p, q) = \mathrm{diam}(X)$ (by compactness). Then defining $\mu = \frac{1}{2}(\delta_p + \delta_q) \in \mathfrak{prop}(X$ gives $I(\mu, \mu) = \frac{1}{2}\,\mathrm{diam}(X)$. Hence $\mathrm{xt}(X) \geq \frac{1}{2}\,\mathrm{diam}(X)$. That $\mathrm{xt}(X) \leq \mathrm{diam}(X)$ since the integrand in $I(\mu, \mu)$, (4.7), is bounded by $\mathrm{diam}(X)$ and the total mass is 1. By compactness of X there is a measure μ realizing $\mathrm{xt}(X)$, Proposition 24. Then $\mathrm{xt}(X) = \mathrm{diam}(X)$ is only possible if $d(x, y) = \mathrm{diam}(X)$ almost everywhere wrt. $\mu \otimes \mu$. So we must exlclude this possibility:

Suppose first that $\mathrm{supp}(\mu)$ is finite, so that $Y = \mathrm{supp}(\mu)$ is isometric to the leaf space of a star graph $\mathrm{Star}(n, l)$, $n = |\,\mathrm{supp}(\mu)|$, with edge lengths $l = \frac{1}{2}\,\mathrm{diam}(X)$. But for such a space we have $\mathrm{xt}(Y) = \frac{n(n-1)}{n^2}\,\mathrm{diam}(X) < \mathrm{diam}(X)$, c.f. 4.4.

If $\mathrm{supp}(\mu)$ is infinite then almost everywhere wrt. μ implies that $d(x, y) = \mathrm{diam}(X)$ must hold for all $x \neq y$ in an infinite set. But then X is not compact, since we can choose a sequence in $\mathrm{supp}(\mu)$ with no convergent subsequences.

Now for the second statement. Having $\mathrm{exc}(X) = 0$ is the same as having a pair of antipodal points, c.f. chapter 1. Let $p, q \in X$ be the antipodal points, which then realizes $\mathrm{diam}(X)$. Choose the probability measure $\mu_1 = \frac{1}{2}(\delta_p + \delta_q)$. Then as before $I(\mu, \mu) = \frac{1}{2}\,\mathrm{diam}(X)$. Now for any probability measure ν with support $Y \subseteq X$ we have:

$$\mathrm{md}(Y, \{p, q\}) = I(\mu, \nu) = \int_{X \times X} d\,\nu \otimes \mu = \frac{1}{2}\,\mathrm{diam}(X) \tag{4.26}$$

This is because the potential of μ is constant by definition of antipodality: $\mathrm{p}_\mu(x) = \frac{1}{2}(d(p, x) + d(x, q)) = \frac{1}{2}\,\mathrm{diam}(X)$. Then apply Fubini's Theorem.

Let $\nu \in \mathfrak{prop}(X)$ realize $\mathrm{xt}(X) > \frac{1}{2}\,\mathrm{diam}(X)$. Computing $I(\mu-\nu,\mu-\nu)$ we get:

$$I(\mu-\nu,\mu-\nu) = \frac{1}{2}\,\mathrm{diam}(X) + \mathrm{xt}(X) - \mathrm{diam}(X) > 0 \tag{4.27}$$

Hence $X \notin \mathcal{NT}$ if $\mathrm{xt}(X) > \frac{1}{2}\,\mathrm{diam}(X)$ and $\mathrm{exc}(X) = 0$.

The other direction is true in general: $\mathrm{xt}(X) = \frac{1}{2}\,\mathrm{diam}(X) \implies \mathrm{exc}(X) = 0$, see [10] Prop. 1.12. □

Remark 22. We could improve the statement in the theorem above to: *having small excess is the same as having small extent (i.e. close to $\frac{1}{2}$ diam X), if X is of negative type*.

For a Riemannian manifold $\mathrm{exc}(M) = 0$ implies that M is a *twisted sphere*. The morale is: *A space of negative type which looks like a sphere, in the sense that it has small excess, cannot be too "fat"*. Here "fat" is supposed to mean, that the "equator" has large diameter. We shall see later, that a space of negative type cannot be too "slim" either.

Using the theorem above we will give examples of some interesting compact length spaces which are not of negative type; in a more positive interpretation it can also be seen as an indication of how to get examples of negative type spaces.

Example 14. Recall that the double of a space X with boundary[6] $\partial X \subset X$ is the set: $\mathrm{db}(X) := X \times \{0,1\}/\sim$, where points on "opposite sides" $(p,0)$, $(p,1)$ are identified iff $p \in \partial X$. The distance on X is extended to $\mathrm{db}(X)$ by

$$d((p,0),(q,1)) := \inf\{d(p,r) + d(r,q) \mid r \in \partial X\}$$

Let $D^n_\kappa(r)$ be a disc in $\mathbb{M}(n,\kappa)$:

$$D^n_\kappa(r) = \{\mathrm{p} \in \mathbb{M}(n,\kappa) \mid d(p,q) \le r\} \text{ centered at some } q \in \mathbb{M}(n,\kappa)$$

We will require that $r \le \frac{\pi}{2\sqrt{\kappa}}$ if $\kappa > 0$, since otherwise $D^n_\kappa(r)$ is not convex, and hence not a length space. The double disc $\mathrm{db}(D^n_\kappa(r))$ is obtained by doubling and identifying along the sphere

$$\partial D^n_\kappa(r) = S^n_\kappa(r) = \{p \in \mathbb{M}(n,k) \mid d(p,q) = r\}$$

It is easy to see that in all cases the center on “one side” q is antipodal to the center on the “other side” $\tilde{q}$. Hence $\mathrm{exc}(\mathrm{db}(D^n_\kappa(r)) = 0$. For $\kappa > 0$ and $r = \frac{\pi}{2\sqrt{\kappa}}$ we have $\mathrm{db}(D^n_\kappa(r)) = \mathbb{S}(n,\kappa)$, which we know is of negative type. But otherwise:

$\mathrm{db}(D^n_\kappa(r))$ is not of negative type for all $\kappa \in \mathbb{R}$ and all $r > 0$ (with $r < \frac{\pi}{2\sqrt{\kappa}}$ for $\kappa > 0$).

To see this, just note that $\mathrm{diam}(\mathrm{db}(D^n_\kappa(r))) = 2r = \mathrm{diam}(D^n_\kappa(r))$ and $\mathrm{xt}(\mathrm{db}(D^n_\kappa(r)) \ge \mathrm{xt}(D^n_\kappa(r)) > r$ since $\mathrm{exc}(D^n_\kappa(r)) > 0$.

For $\kappa > 0$ this gives a family of length spaces, not of negative type, converging to $\mathbb{S}(n,\kappa)$.

[6] which can be taken just to be any compact subset.

Finally we will note the following reformulation of classical conditions for negative type.

Theorem 11. *Let (X, d) be an admissible space. Consider the kernels $S_\lambda(p, q) := \exp(-\lambda d(p, q))$ and $E_r(p, q) := e_{p,q}(r)$, the excess kernel. Let I_{S_λ} and I_{E_r} be the corresponding quadratic forms on $\mathfrak{M}(X)_c$. The following are equivalent:*

1. $X \in \mathcal{NT}$
2. *I_{S_λ} is positive semidefinite for all $\lambda > 0$.*
3. *I_{E_r} is positive semidefinite for one $r \in X$.*
4. *I_{E_r} is positive semidefinite for all $r \in X$.*

Proof. The statement holds for finite subsets, i.e. on $\mathfrak{atom}(X)$. See [7] 9.1, and Proposition 22. Then apply Lemma 17. □

Geometry in $\mathfrak{M}(X)$: We can realize X homeomorphically in $\mathfrak{M}(X)$ in various ways: e.g. the map $X \to \mathfrak{M}(X),\ p \mapsto \delta_p$ is a homeomorphism onto its image because $p_n \to p$ iff $\delta_{p_n} \to \delta_p$ weakly.

This idea also gives a way to prove the constructive part of Theorem 7: Suppose X is of negative type, then for any fixed point r the quadratic form of the excess kernel I_{E_r} is positive semidefinite. Then define the embedding of X into $\mathfrak{M}(X)$ as $p \mapsto \delta_p - \delta_r = v(p)$, so that r is realized as the origin in $\mathfrak{M}(X)$. Then $I_{E_r}(v(p), v(p)) = 2d(p, r) > 0$ for $p \neq r$.

Hence I_{E_r} defines a (pre) Hilbert space structure on a subspace of $\Pi_0(X)_c$ containing the image of X. It is easily checked that with this definition the Hilbert space distance between δ_p and δ_q becomes:

$$d_{\mathcal{H}}(\delta_p, \delta_q)^2 = I_{E_r}(\delta_p - \delta_q, \delta_p - \delta_q) = 2d(p, q)$$

4.6 Variation

This section is mainly a reformulation of the material in [14] using the language of the previous section. Some new insights are added.

Definition 26. Let (X, d) be an admissible space. A continuous curve $\gamma : [0, \epsilon) \to X$, for some $\epsilon > 0$, is called a $\mathcal{V}$-curve through $p \in X$ if $\gamma(0) = p$ and:

$$d(p, \gamma(t)) \geq t \text{ for } t \in [0, \epsilon) \tag{4.28}$$

The set of $\mathcal{V}$-curves through p will be denoted $\mathcal{V}_p$.

The definition of a $\mathcal{V}$-curve is off course designed to mimic a regular curve in a Riemannian manifold M or a geodesic in a length space. We are primarily (only) interested in such spaces and subsets of these, so why not stick to geodesics? The reason is that the $\mathcal{V}$-curve concept makes sense also for irregular, non convex subsets with the extrinsic metric.

Definition 27 (Criticality Index). Let $f : X \to \mathbb{R}$ be a function on an admissible space, and let p be a local maximum of f. The criticality index of f at p, $\mathrm{crind}(f, p)$, is defined as:

$$\mathrm{crind}(f, p) := \text{the infimum of those } \omega \in \mathbb{R}_+ \text{ satisfying}$$

$$\forall \gamma \in \mathcal{V}_p\, \exists c > 0,\ \alpha > 0 :\ f(\gamma(t)) \leq f(p) - ct^{\omega} \text{ for } t \in (0, \alpha)$$

If p is a local minimum of f, define $\mathrm{crind}(f, p) := \mathrm{crind}(-f, p)$.

That a maximum of a function has criticality index ω means that, for all $\epsilon > 0$ f decreases faster than $d^{\omega+\epsilon}$ close to p in every "direction". Note that by the logic of the definition $\mathrm{crind}(f, p) = 0$ if $\mathcal{V}_p = \emptyset$.

For a smooth function $f : \mathbb{R} \to \mathbb{R}$ it is clear by Taylor theory that $\mathrm{crind}(f, p)$ is an even natural number. This generalizes to higher dimensions and manifolds with "sufficiently nice" distances. In contrast to the differentiable case we have e.g.
$\mathrm{crind}(x \mapsto |x|, 0) = 1$ and $\mathrm{crind}(x \mapsto |x|^{\omega}, 0) = \omega$.

Distance Functions Since the distance kernel on a Riemannian manifold M will be of primary interest, we will need to discuss critical points of distance functions of the form $d(\cdot, p)$. Given a point $p \in M$, we use C_p to denote the *cut locus* of p, c.f. [5]. As in [15] we will use $\Lambda_p(q) \subset T_q X$ to denote the set of directions of minimal geodesics from q to p. Then a point $q \in C_p$ is called a *critical point* of $d(\cdot, p)$ if 0_q is contained in the convex hull of $\Lambda_p(q)$ in $T_q M$. For further discussions on critical points of distance functions see [23].

The following can be proved by first variation techniques, c.f. Lemma 2.1. in [15].

Lemma 18. *Let M be a Riemannian manifold and assume that q is a local maximum of $d(\cdot, p)$. Then* $\mathrm{crind}(d(\cdot, p), q) = 1$ *iff* $\mathrm{span}(\Lambda_p(q)) = T_q M$ *and 0_q is contained in the interior of the convex hull of $\Lambda_p(q)$*

We will now consider extrema of the quadratic form corresponding to kernels of the form $f(d)$.

Theorem 12. *Let (X, d) be an admissible space with a kernel of the form $f(d)$, where $f : \mathbb{R}_+ \to \mathbb{R}$ is a continuous function, which has a local minimum at $x = 0$. Consider a distribution $\mu = \alpha\delta_p + \nu \in \mathfrak{M}(X)_c$ with $\nu(p) = 0$ and $\alpha > 0$. In each of the following situations:*

- *μ realizes* $\mathrm{xt}(X, f(d))$.

- *μ realizes* $\mathrm{nt}(X,\ f(d))$ *and* $|\,\mathrm{supp}(\nu)| > 1$*, i.e.* ν *is not a single atom.*

we have the conclusion:

$$\underline{\mathrm{p}_\nu \text{ has a global maximum at } p \text{ and } \mathrm{crind}(\mathrm{p}_\nu, p) \le \mathrm{crind}(f, 0)}$$

Proof. Assume that $\mu = \alpha\delta_p + \nu$ realize one of the relevant sup's We will prove the assertion using two different kinds of variations:

Global variation, moving the atom:

Consider the distribution $\mu_q = \alpha\delta_q + \nu$ for $q \in X$. We have $I(\mu_q, \mu_q) = \alpha^2 I(\delta_q, \delta_q) + I(\nu, \nu) + 2\alpha I(\delta_q, \nu) = \alpha^2 f(0) + I(\nu, \nu) + 2\alpha \mathrm{p}_\nu(q) = \text{constant terms} + 2\alpha \mathrm{p}_\nu(q)$ We see that this produces distributions with larger I-value than $\mu_p = \mu$, unless $\alpha\mathrm{p}_\nu$ has a global maximum at $q = p$. μ_q has the same amount of algebraic mass as μ, i.e. $\mu_q(X)$ is constant. This settles the global max assertion in the case of $\mathrm{xt}(X,\ f(d))$.

In the case of $\mathrm{nt}(X,\ f(d))$ it is relevant whether mass "cancels out", which is possible if ν contains atoms of opposite sign. This will give distributions with smaller absolute mass (norm) , and since the sup is taken over distributions with norm 2, this will have to be considered. Since $\nu \neq \delta_{q_0}$ for any q_0, we have $\mu \neq \delta_p - \delta_{q_0}$. Then for all $q \in X : \mu_q \neq 0$, hence $0 < |\mu_q\| \le \|\mu\| = 2$. Assuming that p is not a global maximum of p_ν, we can find a q s.t. $I(\mu_q, \mu_q) > I(\mu, \mu)$. Since $\mu_q \neq 0$, we can multiply μ_q by $\frac{2}{\|\mu_q\|} \ge 1$, thus producing a distribution in the relevant set with energy not less than $I(\mu_q, \mu_q)$; this is impossible. Hence p is a global max of p_ν.

Local variation, splitting the atom:

Let $\gamma : [0, \epsilon) \to X$ be a $\mathcal{V}$-curve with $\gamma(0) = p$. Define the distribution

$$\mu_t = \frac{1}{2}\alpha\delta_{\gamma(t)} + \frac{1}{2}\alpha\delta_p + \nu \tag{4.29}$$

Then $\mu_0 = \mu$ and the total algebraic mass is unchanged $\mu_t(X) = \mu(X)$ and hence also the norm in the case of $\mathrm{xt}(X)$. It is clear that also in the other case we have $\mu_t \neq 0$ hence $0 < \|\mu(t)\| \le 2$. If the variation increases the energy, a scaling of μ_t by $\frac{2}{\|\mu_t\|}$ cannot decrease the value. The variation $t \mapsto \mu_t$ is a variation in one of the relevant subsets $\mathfrak{prop}(X)_c$ or $\Pi_0(X)_c \cap \mathfrak{B}(2) \setminus \{0\}$.

We have:

$$\begin{aligned} I(\mu_t, \mu_t) = 2\frac{\alpha^2}{4} I(\delta_{\gamma(t)}, \delta_p) + 2\frac{\alpha}{2} I(\delta_{\gamma(t)}, \nu) + 2\frac{\alpha}{2} I(\delta_p, \nu) + \\ I(\nu, \nu) + \frac{1}{4}(I(\delta_p, \delta_p) + I(\delta_{\gamma(t)}, \delta_{\gamma(t)})) = \\ \underbrace{\frac{\alpha^2}{2} f(d(\gamma(t), p))}_{first} + \underbrace{\alpha \mathrm{p}_\nu(\gamma(t))}_{second} + \text{constant terms} \end{aligned} \tag{4.30}$$

Since γ is a $\mathcal{V}$-curve the first term above will increase at least as $ct^{\omega+\eta}$, for $\eta > 0$ and $\omega = \mathrm{crind}(f, 0)$. Since $t = 0$ gives a maximum, the second term must decrease at least as fast. This is true for any $\mathcal{V}$-curve γ and any $\eta > 0$, hence the assertion follows by the definition of criticality index. □

We can add:

Addendum 1. If the extremal distribution in the case of $\mathrm{nt}(X, f(d))$ is $\mu = \delta_p - \delta_q$ for some $q \neq p$, then the conclusion in Theorem 12 holds if

$$\inf\{d(p,q) | p \neq q\} = 0 \text{ and } f \text{ is continuous.}$$

Proof. In this case $\mathrm{p}_\nu = -2f(d_q)$ and the energy is $2f(0) - 2f(d(p,q))$. This obtains a maximum, when p is such that $f(d(p,q))$ is minimal. Consider the set $A = d(X,X) \subseteq \mathbb{R}_+$. Hence $d(p,q)$ must realize the minimum of f on $A \setminus \{0\}$. The global minimum of f on A must then be either at $x = 0$ or at $d(p,q)$. But if $x = 0$ is a unique minimum in A, the minimum on $A \setminus \{0\}$ is only realized if 0 is an isolated point in A, which means that X is discrete with all nontrivial distances bounded away from zero. □

What Theorem 12 says is that a maximal distribution cannot have an "isolated" atom $\mu = \alpha\delta_p + \nu$, unless the potential p_ν has a singularity at p which looks at least as bad as the singularity of f at $x = 0$, from the point of view of differentiability.

We already know this from Lemma 16 in the case of realizations of $I_k(X, f(d))$: If $\mu = \alpha\delta_p + \nu$, then

$$\mathrm{p}_\nu = \mathrm{p}_\mu - \alpha \mathrm{p}_{\delta_p} = \mathrm{const} - \alpha f(d(\cdot, p)), \tag{4.31}$$

which is precisely as critical as $f(d(\cdot, p))$ at p.

Here is another result describing the properties of a maximal distribution; this is inspired by Theorem 1 in [1].

Theorem 13. *Let X be an admissible space with a continuous kernel ϕ.*

- *If $\mu \in \mathfrak{prop}(X)_c$ realizes $\mathrm{xt}(X, \phi)$ then $\mathrm{p}_\mu(q) = \sup_X(\mathrm{p}_\mu) = \mathrm{xt}(X, \phi) < \infty$ for all $q \in \mathrm{supp}(\mu)$.*
- *If $\mu = \mu^+ - \mu^- \in \Pi_0(X)_c \cap \mathfrak{S}(2)$ realizes $\mathrm{nt}(X, \phi)$ then $\mathrm{p}_\mu(q) = \sup_X(\mathrm{p}_\mu) < \infty$ for all $q \in \mathrm{supp}(\mu^+)$ and $\mathrm{p}_\mu(q) = \inf_X(\mathrm{p}_\mu) > -\infty$ for all $q \in \mathrm{supp}(\mu^-)$.*

Proof. The first statement can be proven exactly as in [1], hence we will concentrate on the $\mathrm{nt}(X, \phi)$ case which is very similar.

Consider $q \in \mathrm{supp}(\mu^+)$ and let $r \in X$ be any other point. For a compact neighborhood K of q, define the distribution that "moves positive mass" to r:

$$\nu_K(A) := \mu^+(K)\delta_r(A) - \mu^+(A \cap K), \tag{4.32}$$

for $A \subseteq X$. Then $\nu_K \in \Pi_0(X)_c$ and we have $\|\mu + \epsilon\nu_K\| \le \|\mu\|$ for $\epsilon \in [0,1]$. "The amount of mass created equals the amount moved". A calculation reveals:

$$\begin{aligned} I(\mu,\nu) = \int_X \mathrm{p}_\mu\, \nu &= \mu^+(K)\mathrm{p}_\mu(r) - \int_K \mathrm{p}_\mu\, \mu^+ \\ &\ge \mu^+(K)\mathrm{p}_\mu(r) - \mu^+(K)\sup_K(\mathrm{p}_\mu) = \mu^+(K)(\mathrm{p}_\mu(r) - \sup_K(\mathrm{p}_\mu)) \end{aligned} \tag{4.33}$$

Hence if $\mathrm{p}_\mu(r) > \mathrm{p}_\mu(q)$ then by continuity of p_μ, we can choose K sufficiently small, so that $\sup_K(\mathrm{p}_\mu) < \mathrm{p}_\mu(r)$ and the expression above becomes positive. But this conflicts with Lemma 16.

The inf case is treated similarly by moving negative mass (or by considering $-\mu$). □

Remark 23 (Geometric/Algebraic Variations). Note that the variation in Theorem 12 moves mass around continuously in X, while the variation in the theorem above is continuous in $\mathfrak{M}(X)$, but in X the mass "tunnels" from K to r. One could define a variation of the first kind as a *geometric variation* and the other kind as an *algebraic variation*.

4.7 Applications

We have seen, that any compact metric space X has realizations of $\mathrm{xt}(X,\phi)$ and $\mathrm{nt}(X,\phi)$ (if this quantity is nonzero), when ϕ is a continuous kernel. Here we shall give some applications of the results of the previous section to the properties of such maximal distributions.

Here is a first simple observation regarding realizations of maximal energies with respect to the distance kernel:

Proposition 31. *Let X be a compact Riemannian manifold, then for any finitely supported distribution $\mu \in \mathfrak{atom}(X)$ realizing either $\mathrm{xt}(X)$ or $\mathrm{nt}(X)$ we have: $\mu(p) \neq 0$ implies that $|\mu|(C_p) \neq 0$, there must be at least one atom on the cut locus of p.*

Proof. It is clear from Theorem 12 that for a maximal distribution of the form $\alpha\delta_p + \nu$, the potential p_ν is not differentiable at p. But p_ν is a sum of distances from $\mathrm{supp}(\nu)$, so differentiability of p_ν can only break down when p is on the cut locus of at least one of the points in $\mathrm{supp}(\nu)$, hence at least one of these is a cut point of p. □

In connection with realizations of extent, the classical concept *subharmonicity* turns out to be important. Here we shall just define a sufficiently weak version of this concept, with some immediate applications.

Definition 28. An admissible metric space X is defined to be *distance regular* if it has Hausdorff dimension $k \in [1,\infty)$ and for every $p \in X$ there is a $R_p > 0$ such that $S(p,r) := \{q \in X \mid d(p,q) = r\}$ is compact and has Hausdorff dimension $k-1$ for all $r \in (0, R_p)$.

A continuous function $f : X \to \mathbb{R}$ on a distance regular space is said to be subharmonic if for every $p \in X$, there is a $r_p > 0$ such that $S(p,r)$ is nonempty, compact, of Hausdorff dimension $k-1$ and:

$$\int_{S(p,r)} f\,\mathcal{H} \geq \mathcal{H}(S(p,r))\,f(p), \quad \text{for every } r \in (0, r_p) \tag{4.34}$$

f is called *strictly subharmonic*, if we have strict inequality above for $r \in (0, r_p)$. Here $\mathcal{H}$ denotes $k-1$-dimensional Hausdorff measure.

Example 15. Riemannian manifolds are distance regular. Geometrized graphs (as defined in section 2.6) and also more general locally finite simplicial complexes, with a length metric, are distance regular.

We immediately have:

Lemma 19. *The set of subharmonic functions form a cone: $f + \alpha g$ is subharmonic if f, g are subharmonic and $\alpha \geq 0$. If $\{f_n\}$ is a sequence of subharmonic functions and $f_n \to f$ uniformly then f is subharmonic.*

And then off course:

Proposition 32. *Let ϕ be a continuous kernel on a distance regular space X. If the atomic potentials $\mathrm{p}_{\delta_p} = \phi(\cdot, p) : X \to \mathbb{R}$ are subharmonic, then for every positive measure $\mu \in \mathfrak{M}(X)_c^+$ the potential p_μ is subharmonic.*

Proof. It follows from the lemma above that every finitely supported measure $\mu \in \mathfrak{atom}(X)^+$ has subharmonic potential. But such measures are weakly dense in $\mathfrak{M}(X)_c$, and if $\mu_n \to \mu$ weakly, with $\mathrm{supp}(\mu_n) \subseteq \mathrm{supp}(\mu)$ then $\mathrm{p}_{\mu_n} \to \mathrm{p}_\mu$ uniformly on every compact subset, by Lemma 14. □

We have almost by definition, proven as usual:

Lemma 20 (Maximum Principle). *If $f : X \to \mathbb{R}$ is a subharmonic function on a distance regular space, then f is constant on a neighborhood of any local maximum. Hence if f has a global maximum, then f is constant.*

Then we have similarly to Theorem 3 in [1]:

Theorem 14. *Let X be a subset of a distance regular space Y, and let ϕ be a continuous kernel on Y such that the atomic potentials $\phi(\cdot, p)$ are subharmonic, then a realization of* $\mathrm{xt}(X, \phi)$, $\mu \in \mathfrak{prop}(X)$, *can only have support on ∂X unless* p_μ *is constant in the interior of X.*

Proof. The interior of X is again distance regular. By Theorem 13 p_μ must have a global maximum (over X) at a point of the support. Hence if μ has support in the interior of X, then p_μ is constant in the interior by the maximum principle. □

Remark 24. One way of introducing a "Laplacian" in this general setting would be:

$$\triangle_\omega f(p) := \liminf_{r\to 0_+}\left[\frac{1}{r^\omega}\Big(\frac{1}{\mathcal{H}(S(p,r))}\int\limits_{S(p,r)} f\mathcal{H} - f(p)\Big)\right] \tag{4.35}$$

This gives a "Laplacian" for each $\omega > 0$. And for a subharmonic function and $p \in X$ $\inf\{\omega|\triangle_\omega f(p) > 0\}$, gives a measure of "how subharmonic" f is at p.

It follows from curvature comparison theory, as in [23] chapter 6, that $d(\cdot,\ p)$ is strictly subharmonic if M is an Hadamard manifold (of dimension at least 2). In order to prove that potentials of distributions in $\mathfrak{prop}(M)_c$ are strictly subharmonic, and hence cannot be locally constant, we would have to give an argument that the "Laplacian" of $d(\cdot,\ p)$ is bounded away from zero, and that this property is preserved under convex linear combinations and uniform limits. This could easily be done.

Corollary 11. *Let X be a compact subset of an Hadamard manifold M, then a realization of* $\mathrm{xt}(X)$ *can only have support on ∂X.*

Proof. For $n \geq 2$ we appeal to the remark above for strict subharmonicity. For a compact subset of $\mathbb{R}^1$, the maximal distribution is realized by placing an atom of mass $\frac{1}{2}$ at $\sup(X)$ and $\inf(X)$; this follows from [1]. ☐

In the other extreme we have the geometrized weighted trees, with curvature zero on edges and infinite negative curvature in branch points. It is easily checked explicitly, that an atomic potential $d(\cdot,\ p)$ is strictly subharmonic in a branch point (if we assume that all branch points have degree ≥ 3), and harmonic otherwise on the edges; except for when we are at a *leaf*.

It follows that potentials are subharmonic in the interior of the tree, or everywhere if we consider a larger tree. But to show strict subharmonicity of potentials in branch points, we will again have to appeal to a "strictly positive laplacian"- argument. We will omit the details here.

Corollary 12. *Let X be a compact subset of geometrized weighted tree $\tilde{T}$, then a realization of* $\mathrm{xt}(X)$ *can only have support on the boundary ∂X. Hence a maximal distribution is finitely supported and unique by strictly negative type of $\tilde{T}$.*

This then also holds for a weighted tree $T = (V, E, w)$ with the path distance on the vertex set V: a distribution realizing $\mathrm{xt}(V)$ can only have support in the set of *leaves* of T. A result which could off course be proven with less drastic methods.

There are many further connections between harmonicity, extent, mean distance and negative type, that need to be investigated further. And there are many kernels besides the direct distance kernel, e.g. modifications as $\mathbf{c}_\kappa(d)$, $\exp(d)$ etc. that should be of interest.

Also note, that we have not discussed differentiability properties of potentials on manifolds. This could also be done…

Negative Type and Closed Geodesics

In this subsection we will show that a compact length space of strictly negative type and that a compact Riemannian manifold of negative type must be simply connected, if the dimension is at least 2. Hence in the following X will denote a compact length space, and we always consider the distance kernel d.

For a tuple of four points $x = (p_0, p_1, p_2, p_3) \in X^4$, consider the distribution:

$$\mu_x := \frac{1}{2}(\delta_{p_0} - \delta_{p_1} + \delta_{p_2} - \delta_{p_3}) = \frac{1}{2}\sum_{i=0}^{3}(-1)^i \delta_{p_i} \tag{4.36}$$

Then $\mu_x \in \Pi_0(X)$ and we know from Proposition 23 that all 4-point spaces are in $\mathcal{NT}$ and in $\mathcal{SNT}$, unless they have two antipodal pairs (with respect to the 4-point space). Hence we always have $I(\mu_x, \mu_x) \leq 0$. It is instructive to write out $I(\mu_x, \mu_x)$ explicitly:

$$I(\mu_x, \mu_x) = \frac{1}{2}(d_{02} + d_{13} - d_{01} - d_{03} - d_{12} - d_{23}) \tag{4.37}$$

Comparing this with the definition of 0-hyperbolicity, Definition 18, we see that for such a space, reassuringly, the sum is negative. Playing around with the expression above and using the triangle inequality it is not difficult to see, that the sum is zero if and only if p_0, p_2 and p_1, p_3 are antipodal (or all terms are zero).

A configuration $x = (p_0, \ldots, p_3) \in X^4$ is called nontrivial if $\mu_x \neq 0$, which means that x is not in the diagonal of X^4 (i.e. all 4 elements equal). We then immediately have:

Proposition 33. *Let X be a compact length space, and consider the function*

$$\mathrm{nt}_4 : X^4 \to \mathbb{R} \quad , x = (p_0, p_1, p_2, p_3) \mapsto I(\mu_x, \mu_x), \tag{4.38}$$

where $\mu_x := \frac{1}{2}\sum_{i=0}^{3}(-1)^i \delta_{p_i}$. Then $\mathrm{nt}_4(x) \leq 0$ for all $x \in X^4$ and a nontrivial zero exists iff there is a closed geodesic $\gamma : \mathbb{R} \to X$ of period $2L$ and two points $\gamma(s_0), \gamma(s_1)$ such that the subarcs

$$\gamma([s_0 + nL, s_0 + (n+1)L]),\ \gamma([s_1 + nL, s_1 + (n+1)L]) \tag{4.39}$$

are minimal for $n \in \{0, 1\}$ (hence for all $n \in \mathbb{Z}$).

Proof. That a nontrivial zero exists means that we have a nontrivial configuration $x = (p_0, p_1, p_2, p_3) \in X^4$ with two antipodal pairs, and by the choice of masses these must be $\{p_0, p_2\}, \{p_1, p_3\}$. Connect the points by 4 minimal geodesics in the following sequence $\gamma_{01}, \gamma_{12}, \gamma_{23}, \gamma_{30}$, where $\gamma_{i,i+1}$ connects p_i and p_{i+1} modulo 4. Then since p_{i+1} is in between p_i and p_{i+2} modulo 4, the curve $\gamma_{i,i+1} \cup \gamma_{i+1,i+2}$ will be minimal hence a geodesic. Then the entire curve fits together to form a closed geodesic, which is seen to satisfy the requirement.

The other way around: if γ is a geodesic satisfying the requirements, then just choose $p_0 = \gamma(s_0)$, $p_2 = \gamma(s_0 + L)$, $p_1 = \gamma(s_1)$, $p_3 = \gamma(s_1 + L)$. Then we have two pairs of antipodal points on γ, which does give a zero of nt_4. □

Hence if X has a closed geodesic containing two pairs of points, such that the distance restricted to these points looks like two pairs of antipodal points on $\frac{L}{\pi}\mathbb{S}^1$, then X is not of strictly negative type. In fact a much stronger existence result holds if X is not simply connected:

Lemma 21. *In a compact length space X which is not simply connected, there is among the closed curves which are nontrivial with respect to free homotopy a curve of minimal length. This curve γ is a simply closed geodesic, and the image $\gamma(\mathbb{R})$ is as a metric subspace isometric to $\frac{L}{\pi}\mathbb{S}^1$, where $2L$ is the period of γ. Furthermore if X is a Riemannian manifold, then for every s, the two arcs of γ are the only minimal geodesics connecting $\gamma(s)$ and $\gamma(s+L)$.*

Proof. For the existence of the minimal, simply closed geodesic, see e.g. [5] Theorem 4.12 and p. 214-215. Let $\gamma : \mathbb{R} \to X$ be this geodesic, and let $2L > 0$ be the period, i.e. $\gamma(t+2L) = \gamma(t)\,\forall t \in \mathbb{R}$.

γ will have to minimize distance between $\gamma(t)$ and $\gamma(t+s)$ for $0 \le s \le L$, that is $d(\gamma(t), \gamma(t+s)) = s$. For if there were a strictly shorter connection ω between $\gamma(t)$ and $\gamma(t+s)$, two closed curves shorter than γ could be constructed by ω and the two arcs of γ. These two curves would have to be homotopically trivial, and hence this would also be true for γ, a contradiction. Hence the image of γ is isometric to a circle of length $2L$.

In the Riemannian case the same argument can be repeated, were we only require ω to be *another* minimizing geodesic connecting $\gamma(t)$ and $\gamma(t+s)$. This would give two nonsmooth closed curves of same length as γ, and by a first variation argument each of these are homotopic to a strictly shorter closed curve. Hence each would have to be homotopically trivial, and then as before this would hold for γ. □

Then from the proposition above we have:

Corollary 13. *A compact length space of strictly negative type is simply connected.*

As examples of compact length spaces of strictly negative type we have the *finite geometrized trees*, which reassuringly are simply connected, while a geometrized graph that contains a closed circuit is not and hence cannot be in $\mathcal{SNT}$.

For a compact Riemannian manifold, we have the stronger statement given in Theorem 15 below.

Lemma 22. *Let X be a compact Riemannian manifold of negative type and assume that $\mathrm{nt}_4(x) = 0 = \mathrm{nt}(X)$, for some nontrivial configuration $x = (p_0, p_1, p_2, p_3) \in X^4$. Then for every point p_i the "antipodal" p_{i+2} (modulo 4) is a local maximum of $d(\cdot, p_i)$ with $\mathrm{crind}(d(\cdot, p_i), p_{i+2}) = 1$.*

Proof. We then have from Proposition 33, that the four points of x lie on a closed geodesic γ, with minimal subarcs as described.

Fix a point of x, e.g. p_2. The potential of the other atoms $\nu = \frac{1}{2}(\delta_{p_0} - \delta_{p_1} - \delta_{p_2})$ is $\mathrm{p}_\nu = \frac{1}{2}(d(\cdot, p_0) - d(\cdot, p_1) - d(\cdot, p_3))$. By Theorem 12, p_ν must have a maximum of criticality index 1 at q.

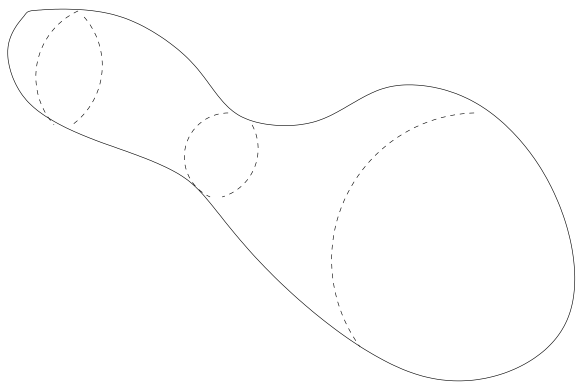
But p_2 is inside the injectivity radius from p_1 and p_3, hence the sum $-(d(\cdot, p_1) + d(\cdot, p_3))$ is smooth at p_2 and in fact has vanishing gradient, since p_1 and p_3 are in opposite directions. This implies that p_ν can only have a maximum of criticality index 1 at p_2 if p_2 is a local maximum of p_2 with criticality index 1. $\square$

That a similar thing does not hold for a compact length space, can be seen by considering e.g. a graph which is a circuit with 4 vertices, with an extra edge attached to one of these vertices. (Perhaps it holds with bounded curvature?)

Theorem 15. *A compact Riemannian manifold X of negative type and dimension at least* 2 *is simply connected.*

Proof. If X is not simply connected, then X contains a *circle* by Lemma 21, which is a homotipacally nontrivial curve of minimal length. This circle then gives a realization of $\mathrm{nt}(X) = \mathrm{nt}_4(x) = 0$ as above. Hence if we exclude that the distance $d(\cdot, p_i)$ can have a local maximum of criticality index 1 at p_{i+2}, then X cannot be of negative type by the previous lemma. But by the last statement of Lemma 21, for every s the "antipodal" $\gamma(s + L)$ must be a *normal cut point* of $\gamma(s)$: $\gamma'(s + L)$ and $-\gamma'(s + L)$ are the only elements of $\Lambda_{\gamma(s)}(\gamma(s + L))$, hence $d(\cdot, \gamma(s))$ does not have a local max of criticality index 1 at $\gamma(s + L)$ by Lemma 18 (go in a direction orthogonal to γ). $\square$

Figure 4.5: A metric on $\mathbb{S}^2$ which is not of negative type.



There are other situations when X contains metric circles and Lemma 22 applies:

Theorem 16. *Let X be a compact Riemannian manifold of negative type and dimension at least* 2*. If $p, q \in X$ realize the injectivity radius, $d(p, q) = \mathrm{inj}(X)$, then p and q are conjugate along some minimal geodesic connecting p and q.*

Proof. If p and q are not conjugate along any minimal geodesic connecting p and q, then it follows from Klingenberg's Lemma, c.f. [5], that p and q lie on a metric circle γ, and furthermore that the arcs of this geodesic are the only geodesics connecting p and q.

But then as before this gives a realization of $\operatorname{nt}(X) = 0$ by a configuration of 4 points. But by Lemma 18, the “antipodal” to a point on this geodesic is not a local maximum of criticality index 1, hence X cannot be of negative type. $\square$

What the preceding discussion shows, is that a Riemannian manifold of negative type cannot be "too slim" in some region, so that we have a closed geodesic which is "almost" a metric circle, such that "antipodal pairs" are not local maxima of the distance function.

Then we can exclude another class of nice Riemannian manifolds from being of negative type:

Corollary 14. *The projective spaces $\mathbb{K}P^n$ are not of negative type for $n \geq 2$, $\mathbb{K} = \mathbb{R}, \mathbb{C}$ and $\mathbb{Q}$, the quarternions.*

Proof. We have $\pi_1(\mathbb{R}\mathrm{P}^2) = \mathbb{Z}_2$, hence $\mathbb{R}\mathrm{P}^2$ is not of negative type. But all the other projective spaces contains $\mathbb{R}\mathrm{P}^2$ as an isometric subset, with the *extrinsic* distance, c.f. [4], [27]. $\square$

Question: We could off course define the nt_n-function as above for n an even number greater than 4. Perhaps the invariants $\operatorname{nt}_n(X) := \sup_X(\operatorname{nt}_n(X))$ could turn out to be interesting. And perhaps they could be used to say something about the higher homotopy or homology groups? Reversing the sign and considering the kernel $-d$, we can interpret $-\operatorname{nt}_n(X)$ as a minimal energy and a configuration realizing $-\operatorname{nt}_n(X)$ as an equilibrium position; which can then be stable or not...

The Sphere

In this subsection we shall describe extremal distributions and their potentials on the round sphere, the only example we have so far of a compact Riemannian manifold of negative type. We will concentrate on the curvature one case, the other cases are obtained from this by scaling; we will here just write $\mathbb{S}^n := \mathbb{S}(n, 1)$.

The cut locus of a point $p \in \mathbb{S}^n$ is exactly the antipode of p. Hence we have from Proposition 31:

Proposition 34. *If $\mu \in \mathfrak{atom}(X)$ is a finitely supported distribution realizing either* $\operatorname{nt}(\mathbb{S}^n)$ *or* $\operatorname{xt}(\mathbb{S}^n)$*, then for every $p \in \operatorname{supp}(\mu)$, the antipode $\sigma_A(p)$ must be in* $\operatorname{supp}(\mu)$.

From the discussion of closed geodesics we already know that $\operatorname{nt}(\mathbb{S}^n) = \operatorname{nt}_4(\mathbb{S}^n) = 0$ is realized by a configuration of 2 antipodal points each of mass $\frac{1}{2}$ together with another pair of antipodal points of mass $-\frac{1}{2}$.

In [10] $\operatorname{xt}(\mathbb{S}^n)$ was calculated to $\frac{\pi}{2}$, realized by a pair of antipodal points each of mass $\frac{1}{2}$. This actually also follows from Theorem 10 since $\operatorname{exc}(\mathbb{S}^n) = 0$.

Since we do not have strictly negative type, there is no guarantee of uniqueness of realizations of $\operatorname{xt}(\mathbb{S}^n)$, and indeed every pair of antipodal points gives one. It is easy to see (as in the proof of Theorem 10) that for such a configuration we have the constant potential $\mathrm{p}_\mu = \frac{1}{2}\pi$. Hence for the 4-point configuration realizing $\mathrm{nt}_4(\mathbb{S}^n) = 0$ we have constant zero potential: $\mathrm{p}_{\mu^+} - \mathrm{p}_{\mu^-} = \frac{\pi}{2} - \frac{\pi}{2} = 0$.

Are there any nonatomic distributions realizing $\mathrm{xt}(\mathbb{S}^n)$? When a space X is of negative type, a convex linear combination of two realizations of $\mathrm{xt}(X)$ gives another. This does suggest:

Proposition 35. *Any distribution on $\mathbb{S}^n$ which is symmetric with respect to the antipodal isometry, $\sigma_A : \mathbb{S}^n \mapsto \mathbb{S}^n$, has constant potential.*

For normalized Riemannian volume measure on $\mathbb{S}^n$ we have: $\mathrm{md}(\mathbb{S}^n) = \frac{\pi}{2}$, *hence this gives a realization of* $\mathrm{xt}(\mathbb{S}^n)$.

Proof. That a distribution $\mu \in \mathfrak{M}(\mathbb{S}^n)$ is symmetric wrt. σ_A implies that $\mathrm{p}_\mu \circ \sigma_A = \mathrm{p}_\mu$. For any $q \in \mathbb{S}^n$ define $\mu_q := \delta_q + \delta_{\sigma_A(q)}$, then the potential of μ_q is constant π. By Fubini's Theorem we have: $\int_X \mathrm{p}_{\mu_q}\, \mu = \mu(\mathbb{S}^n)\pi = \int_X \mathrm{p}_\mu\, \mu_q = \mathrm{p}_\mu(q) + \mathrm{p}_\mu(\sigma_A(q))$, which gives the result.

A simple and brutal integration using polar coordinates would give the result about $\mathrm{md}(\mathbb{S}^n)$. We will use the previous result. Place $\mathbb{S}^n$ with it's n-dimensional normalized volume measure as the equator in $\mathbb{S}^{n+1}$. This distribution is then antipodally invariant and has constant potential. On the equator it is equal to $\mathrm{md}(\mathbb{S}^n)$. But as is easily seen, at a pole it is $\frac{\pi}{2}$. ☐

Observation 7. We see from the proof, that any antipodally invariant distribution of mass 1 has constant potential $\frac{\pi}{2}$.

We then have several interesting realizations of $\mathrm{nt}(\mathbb{S}^n) = I_0(\mathbb{S}^n) = 0$. In fact any antipodally invariant distribution in $\Pi_0(\mathbb{S}^n)$ gives zero energy. This implies e.g. by the section on geometric characterizations of negative type: For any two subspheres $\mathbb{S}^{m_1}$ and $\mathbb{S}^{m_2}$ of $\mathbb{S}^n$:

$$\mathrm{md}(\mathbb{S}^{m_1}) + \mathrm{md}(\mathbb{S}^{m_2}) = \pi = 2\,\mathrm{md}(\mathbb{S}^{m_1}, \mathbb{S}^{m_2}) \implies \mathrm{md}(\mathbb{S}^{m_1}, \mathbb{S}^{m_2}) = \frac{\pi}{2}$$

Mean Distance and Curvature Let X be a compact Riemannian manfiold equipped with its usual volume form, which we normalize so that $\mathrm{vol}(X) = 1$, hence $\mathrm{vol} \in \mathfrak{prop}(X)$. Then clearly $\mathrm{md}(X) \leq \mathrm{xt}(X)$, where the mean distance is taken with respect to vol. And we would expect strict inequality unless X is quite special (quite "round"). As an example consider a topological sphere X which is a "thin fattening" of the interval $[0, 1]$. Then $\mathrm{xt}(X) \approx \frac{1}{2}$ but $\mathrm{md}(X) \approx \frac{1}{3}$.

In [10] the round sphere $\mathbb{S}^n$ is characterized as having maximal extent among n-dimensional Alexandrov spaces of curvature ≥ 1.

A similar statement holds, when extent is replaced by mean distance (with respect to the natural measure, *normalized n-dimesional Hausdorff measure*). This can be proved by Toponogov's Theorem, as in [10]. However it also follows directly from Theorem A in [10] and the proposition above.

An interesting question then presents itself: *What if sectional curvature ≥ 1 is replaced by Ricci curvature $\geq n-1$?* Several things suggests that it still holds, that the round sphere has maximal mean distance among such manifolds, with respect to normalized volume measure…

In Search of Examples, Conclusions

We have shown that a compact Riemannian manifold of negative type and dimension at least 2 must be simply connected, and also that the complex and quarternionic projective spaces, which otherwise are prototypes of simply connected manifolds, are not of negative type. One has to be more creative to find examples. An easy argument using Theorem 12 also shows (see [14]):

Proposition 36. *A Riemannian product manifold $X = X_1 \times X_2 \cdots \times X_k$ is not of negative type if one of the factors is not of strictly negative type. Hence a Riemannian product manifold , where one of the factors is $\mathbb{S}(n,\kappa)$, $n \geq 1$, is not of negative type.*

However first calculations and thoughts seem to support that it is possible to construct simplicial complexes with constant nonpositive curvature on subsimplices, such that the resulting length space is of negative type.

As an example we may consider a *double simplex*, i.e. a length space consisting of two copies of a simplex $\Delta \subset \mathbb{M}(n,\kappa)$, glued together along the boundary, c.f. Example 14. Consider e.g. a *regular simplex* with edge lengths l, $\Delta_\kappa \subset \mathbb{M}(n,\kappa)$. Then for $\kappa \to \infty$ the simplex Δ_κ will converge in Gromov-Hausdorff distance towards a geometrized star graph $\mathrm{Star}(n+1, \frac{l}{2})$. Then also the double $\mathrm{db}(\Delta_\kappa)$ will be close to this star graph and could possibly be of negative type.

It then seems reasonable that a "fattening" of such a space, thus producing some positive curvature, could be of negative type. We know, that a compact manifold of negative type must have enough positive curvature to assure that points realizing the injectivity radius are conjugate. Hence the "fattening" should be done in a careful manner so that one does not introduce metric circles: No matter how close the fattening is to the star graph length space in the Gromov-Hausdorff sense, if it gets to "thin" somewhere so that we have a "forbidden metric circle", then the resulting manifold is not of negative type.

By the results of section 4.6 it is also possible to say something about how maximal distributions should look, and use this as a guide for checking negative type. Consider e.g. a double regular triangle in curvature κ. Here the "critical" points should be the center of mass on each side and the 3 vertices. Placing masses in these 5 points (in the obvious way), it is easily seen that a double triangle is never hypermetric. However it could (and should) be of negative type.[7]

So the claim is, that there should be examples of metrics on $\mathbb{S}^n$ of negative type, which does not have constant curvature. *The round sphere is not a lone soul in the category of compact Riemannian manifolds of negative type*[8].

[7] This example was suggested by Karsten Grove. Computer experiments seem to support negative type…

[8] Is it isolated, or could one deform it to e.g. a manifold of negative type, looking like a drop?

However it is still an interesting question whether negative type has further topological implications, besides for the first homotopy group?

Final Remarks: The "mystery" about the role of negative type in Riemannian geometry has not been solved completely, but hopefully by now one should have more "feeling" for what negative type means geometrically. And at least have seen, that it has connections to many interesting geometric problems. Many of these connections need to be investigated further. . .

Bibliography

[1] G. Björck: *Distributions of positive mass*, Arkiv för Matematik, Bd. 3, nr. 21, 1956.

[2] L. M. Blumenthal: *Theory and Applications of Distance Geometry*, 2nd. ed., Chelsea, New York, 1970.

[3] V. N. Berestovskij: *Spaces with bounded curvature and distance geometry*, Sibirsk. Mat. Zh. 27, no. 1, 197, 1986.

[4] A. Besse: *Manifolds all of whose geodesics are closed*, Springer-Verlag, Berlin-New York, 1978.

[5] I. Chavel: *Riemannian geometry-a modern introduction*, Cambridge University Press, Cambridge, 1993.

[6] F. H. Clarke: *Optimization and nonsmooth analysis*, 2.nd ed., SIAM, Philadelphia, 1990.

[7] M. Deza, M. Laurent: *Geometry of Cuts and Metrics*, Algorithms and Combinatorics 15, Springer-Verlag, Berlin, 1997.

[8] J. Faraut & K. Harzallah: *Distance hilbertiennes invariantes sur un espace homogéne*, Ann. Inst. Fourier 24, 1974

[9] F. R. Gantmacher: *The Theory of Matrices*, Vol. 2, Chelsea, New York, 1959

[10] K. Grove & S. Markvorsen: *New extremal problems for the Riemannian recognition program via Alexandrov geometry*, J. Amer. Math. Soc. 8, no. 1, 1995

[11] U. Haagerup & H. J. Munkholm: *Simplices of maximal volume in hyperbolic n-space*, Acta. Math. 147, No. 1-2, 1981

[12] P. de la Harpe: *Sur les groupes hyperboliques d'après Mikhael Gromov*, Progress in Mathematics 83, Birkhäuser, Boston, 1990.

[13] P. G. Hjorth, P. Lisonek, S. Markvorsen & C. Thomassen: *Finite Metric Spaces of Strictly Negative Type*, Linear Algebra Appl. 270, 1998.

[14] P. G. Hjorth, S. L. Kokkendorff & S. Markvorsen: *Hyperbolic Spaces are of Strictly Negative Type*, Proc. Amer. Math. Soc. 130, No. 1, 2002

[15] J. I. Itoh & M. Tanaka: *The Lipschitz continuity of the distance function to the cut locus*, Trans. Amer. Math. Soc. 353, no. 1, 2001.

[16] J. B. Kelly: *Hypermetric Spaces and metric transforms*, Inequalities II (O. Shisha, Ed.), Academic Press, 1970.

[17] J. B. Kelly: *Combinatorial Inequalities*, Combinatorial Structures and Their Applications, (R. Guy et. al., Ed.), Gordon and Breach, 1970

[18] S. L. Kokkendorff: *Gram Matrix Analysis of Finite Distance Spaces in Constant Curvature*, Mat-Report No. 2002-17 (preprint).

[19] S. Markvorsen: *Analysis on minimal metric graphs in Riemannian manifolds*, Mat-Report No. 2002-5 (preprint).

[20] J. Milnor: *The Schläfli Differential Equality*, Collected papers. Vol. 1. Geometry, Publish or Perish, Houston, 1994.

[21] B. O'Neill: *Semi-Riemannian Geometry With Applications to Relativity*, Academic Press, 1983.

[22] G. K. Pedersen: *Analysis Now*, Graduate Texts in Mathematics 118, Springer-Verlag, New York, 1989

[23] P. Petersen: *Riemannian Geometry*, Graduate Texts in Mathematics 171. Springer-Verlag, New York, 1998.

[24] C. D. Hodgson & I. Rivin: *A characterization of compact convex polyhedra in hyperbolic* 3*-space*, Invent. Math. 111, No. 1, 1993.

[25] I. Rivin: *A characterization of ideal polyhedra in hyperbolic* 3*-space*, Ann. of Math. (2) Vol. 143, No. 1, 1996.

[26] G. Robertson & T. Steger: *Negative definite kernels and a dynamical characterization of property (T) for countable groups*, Ergodic Theory Dynam. Systems 18, 1998.

[27] G. Robertson: *Crofton formulae and geodesic distance in hyperbolic spaces*, J. Lie Theory 8, 1998.

[28] I. J. Schoenberg: *A remark to Maurice Fréchets article.*, Ann. of Math. Vol. 36, No. 3, 1935.

[29] J.-M. Schlenker: *Métriques sur les polyédres hyperboliques convexes* , J. Differential Geom. 48, No. 2, 1998.

[30] J.-M. Schlenker:*Convex polyhedra in Lorentzian space-forms*, Asian J. Math. 5, 2001.

[31] E. Suàrez-Peirò: *A Schläfli differential formula for simplices in semi-Riemannian hyperquadrics*, Pacific J. Math. 194, 2000.